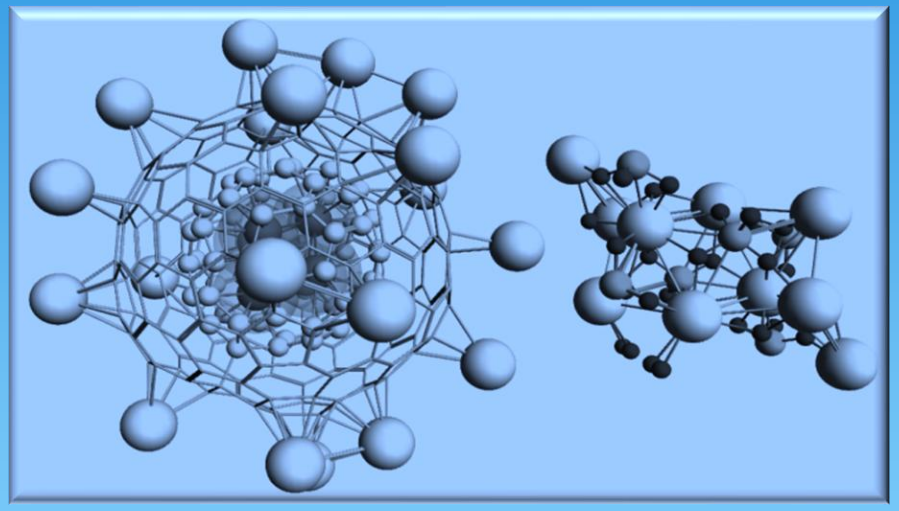
TECNOLOGÍA AVANZADA

NANOTECNOLOGÍA Y MATERIALES FUNCIONALES



NANOCÁPSULAS DE CARBONO CON COMPUESTOS RADIACTIVOS PARA DIRIGIR MEDICAMENTOS A ZONAS ESPECÍFICAS DEL CUERPO

Dr. Alejandro Valderrama

3 de septiembre de 2014

CICATA, IPN

Posgrado en Tecnología Avanzada

UNAM POSGRADO

RESUMEN

1. *Aplicamos supercómputo y con el código para procesamiento en paralelo Quantum Espresso (QE) para los cálculos y el software de procesamiento simple Ámsterdam Density Functional (ADF) para realizar las representaciones.*
2. *Usamos Teoría de Funcional de Densidad Electrónica (DFT) con pseudopotenciales (PP) de conservación de norma Perdew-Burke-Erzerhof (PBE) exch-corr scalar relativistic para realizar relajaciones y Dinámicas Moleculares (MD).*
3. *Simulamos el fullerene C_{60}, conteniendo diferentes cantidades de moléculas de compuestos del yodo radioactivo ^{131}I.*
4. *Los fullerenos con compuestos radioactivos en su interior, presentaron inestabilidad en presencia de átomos de calcio, fósforo y estroncio; que rompieron las nanocápsulas liberando su contenido de yodo radioactivo.*
5. *Simulamos un buckyball multi capa: $C_{60}@C_{180}$.*
   a. *Este nano sistema de dos esferas de carbono concéntricas es estable y tiene una energía mínima en el estado fundamental de – 37.133 keV.*
   b. *El sistema, $C_{60}@C_{180}$ permite almacenar en la esfera interior hasta 3 moléculas de compuestos de yodo radioactivo y adsorber en la superficie de la esfera exterior 20 átomos de calcio.*
   c. *El sistema $[3\#^{131}I@C_{60}@C_{180} + 20Ca]$ es estable y es capaz de interaccionar con otras moléculas con afinidad química con él calcio, como es la de fosfato de calcio cristalino $[Ca_{10}(PO_4)_6(OH)_2]$ que se presenta en los huesos bajo la forma de hidroxiapatita (HA).*

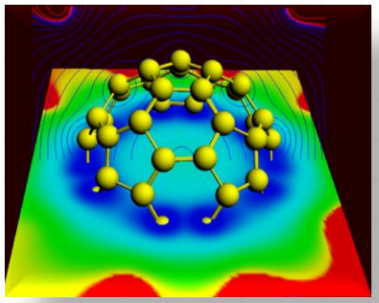
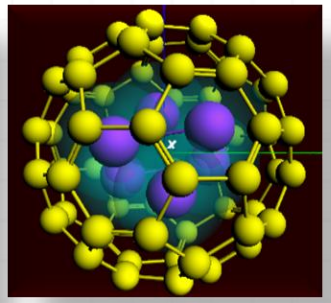
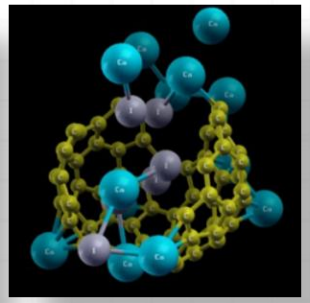
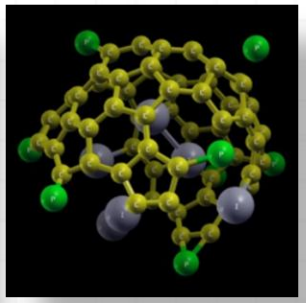
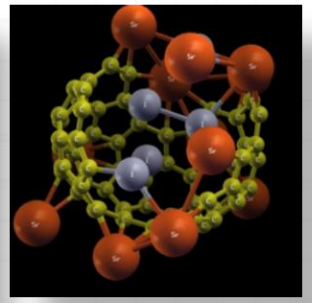
RESUMEN

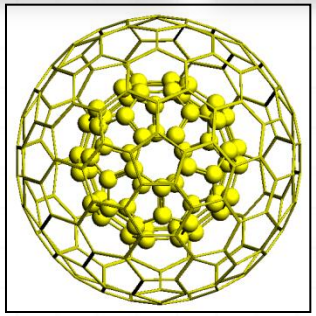
Nuevo Equipo de Supercomputo

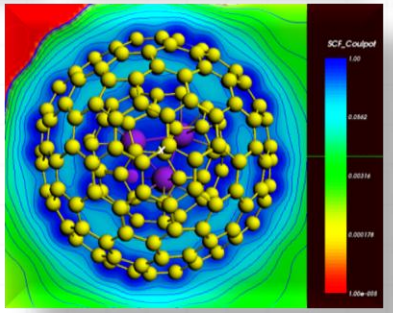
QUANTUM ESPRESSO

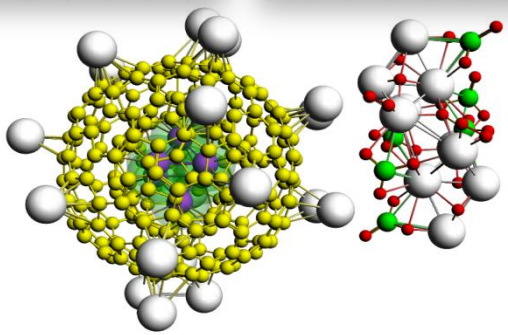
XCrySDen ...
X-window CRYstalline Structures and DENsities

DFT



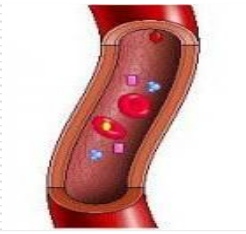


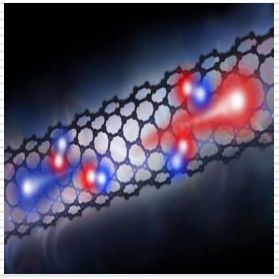


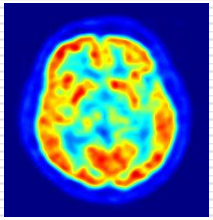
CICATA, IPN

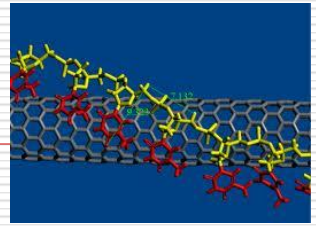
Introducción

- El cáncer es una enfermedad que ataca a nivel celular.
- Actualmente los tratamientos basados en terapias de radiación y quimiofármacos afectan tanto a las células enfermas como a las células sanas por lo que su eficacia es reducida.
- Es necesario estudiar una nueva generación de medicamentos que puedan distinguir a las células enfermas y realizar la medicación de manera localizada.



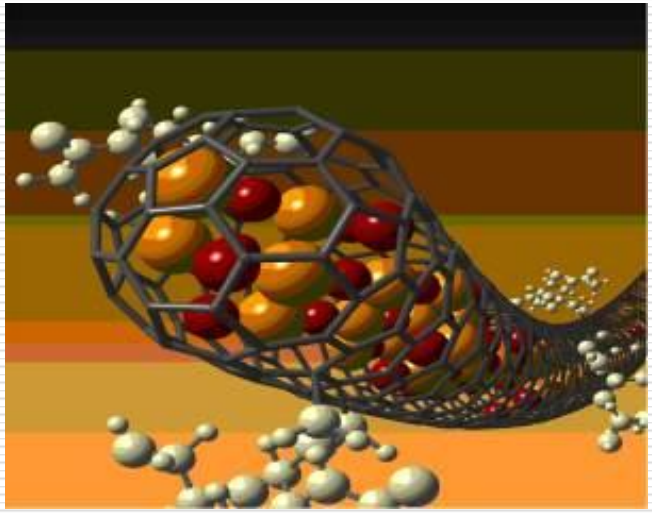






Antecedentes

El Consejo Superior español de Investigaciones Científicas (CSIC), ha logrado desarrollar nanocápsulas de carbono que alojan en su interior un compuesto radiactivo que podría tener una potencial aplicación en el tratamiento de tumores.

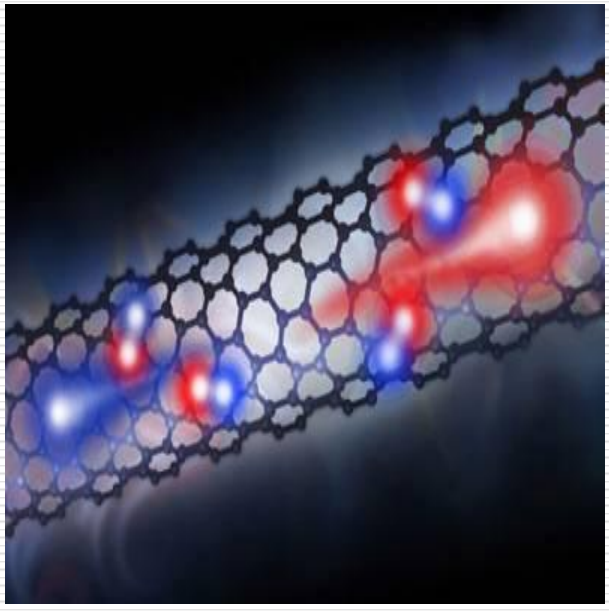


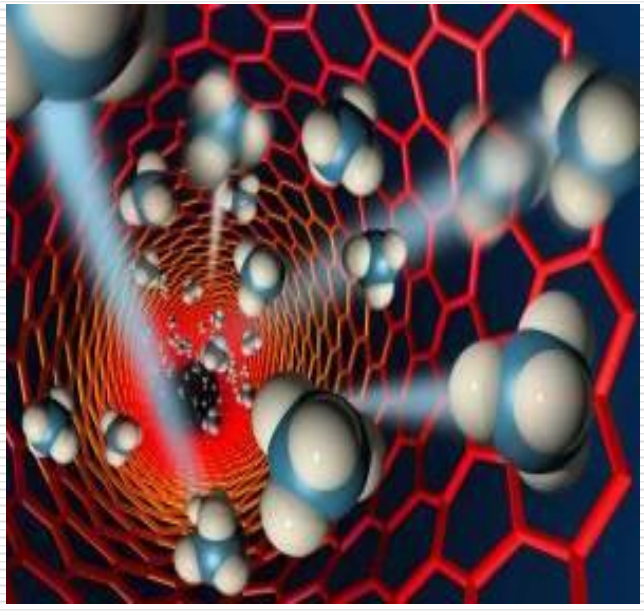
CICATA, IPN

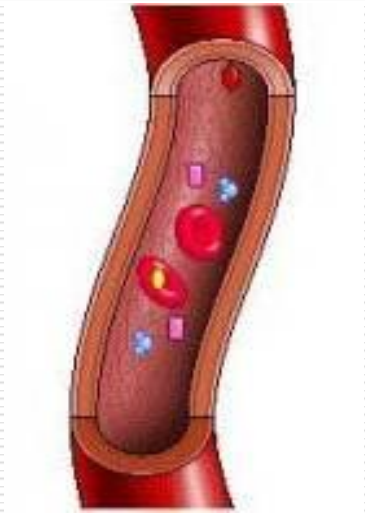
Nanocápsulas de yoduro

Los Yoduros de Sodio y Potasio son compuestos radiactivos extensamente utilizados para el tratamiento de cáncer de tiroides dada la gran afinidad que presentan hacia este órgano.

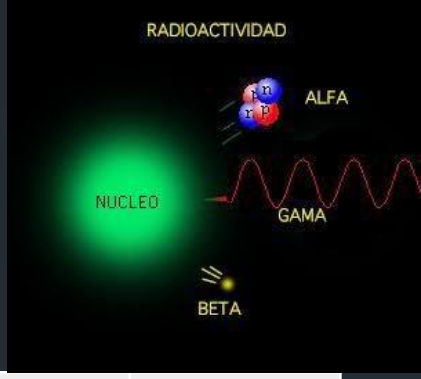
Yoduro de potasio





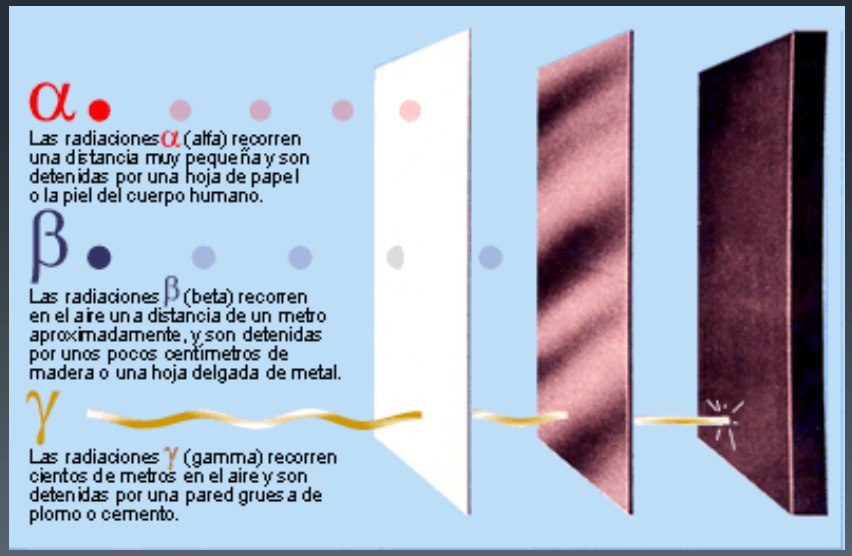


Isótopos estables y radioactivos



Isótopo	Reactividad	Protones	Neutrones	Electrones	Nucleones	Peso atómico	u = g/M
I 129	Estable	53	76	53	129	130.073	126.9045
I 131	8.3 días	53	78	53	131	132.091	
Co 59	Estable	27	32	27	59	59.489	58.9331
Co 60	5.27 años	27	33	27	60	60.497	

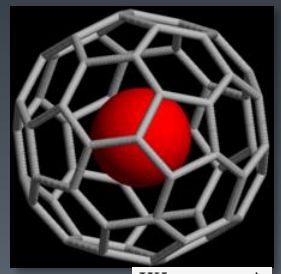
La **energía de desintegración** es la diferencia de energía existente entre las partículas iniciales y las finales de un proceso de desintegración .



Otros Elementos Radioactivos

Los isótopos radioactivos de kriptón y xenón se pueden almacenar y manipular más fácilmente en forma gaseosa.

Representación de una molécula de C_{60} que contiene un átomo de gas noble.

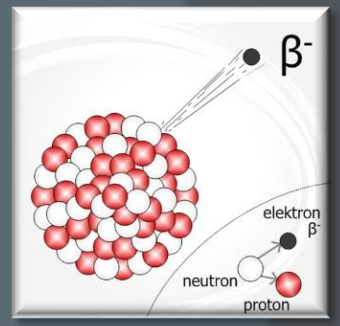


Decaimiento Radioactivo del ^{131}I

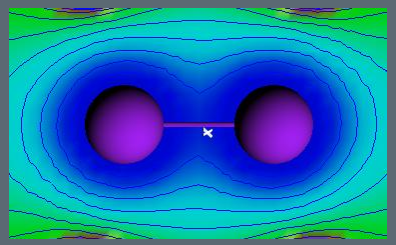
- ^{131}I (78 neutrones) decae con un periodo de 8.0197 días con emisiones beta y gamma.
- Al decaer, el ^{131}I se transforma en ^{131}Xe: $^{131}_{53}\mathrm{I} \rightarrow \beta + {}^{131}_{54}\mathrm{Xe}$
- Esta es la ecuación de la desintegración beta menos de yodo 131:

$$_{53}{}^{131}I \Rightarrow {}_{54}{}^{131}Xe + e^{-} + \nu_e$$

- El yodo 131 se transforma cuando un neutrón se convierte en un protón y un electrón se crea y es expulsado del núcleo, junto con un antineutrino.
- Las emisiones primarias del ^{131}I son 364 keV de radiación gamma (abundancia del 81%) y partículas beta con una energía máxima de 606 keV (abundancia del 89%).



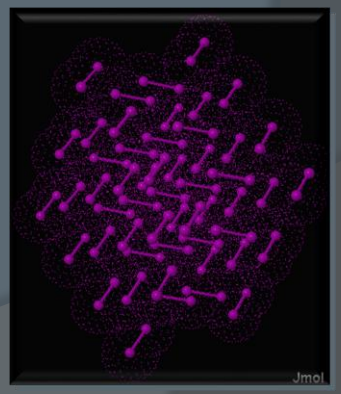
Desintegración


Energía Total = -624.7860 eV

Longitud del enlace ^{129}I - ^{129}I = 2.66 Å
Masa atómica = 126.9045 u
Energía de Enlace LDA = -1.6986104 eV

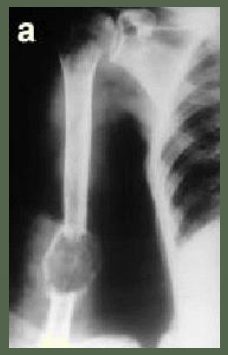
Longitud del enlace ^{131}I - ^{131}I = 2.66 Å
Masa atómica = 132.091 u
Energía de Enlace LDA = -1.6986610 eV

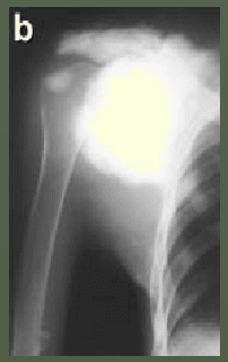
ATOMS	X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1 I.0	0.0000	0.0000	1.3300	53.00	7.00	132.0910
2 I.0	0.0000	0.0000	-1.3300	53.00	7.00	132.0910



Gas de I_2 Molecular

Kambalam
COMPUTO academico UNAM
QUANTUM ESPRESSO
AMD Athlon X2 64
XCrySDen ... X-window CRYstalline Structures and DENsities
intel inside CORE i3
SCH





Isótopos radioactivos usados comúnmente para combatir el cáncer

- **Yodo-131:** Su uso es generalizado para tratamiento de hipertiroidismo y cáncer de tiroides. Vida media de 8.3 días.
- **Fósforo-32:** de gran eficacia terapéutica por la mayor selectividad hacia el tejido tumoral y menor toxicidad por su administración en un corto periodo de tiempo. Vida media de 14 días.
- **Estroncio-89:** capacidad de fijarse las zonas de actividad osteoblástica. Vida media de 50 días.
- **Samario-153:** para el cáncer de mama y próstata. Vida media de 46.3 horas.

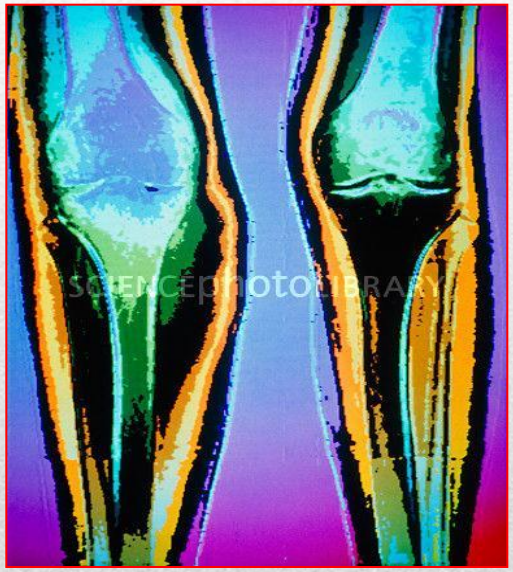
Una de las características propias tanto de tumores sólidos como hematológicos consiste en la frecuente propensión a formar metástasis óseas. Se ha estimado que anualmente mueren 350.000 personas con metástasis óseas en EEUU.

http://www.cfnavarra.es/salud/anales/textos/vol29/n2/colaba.html

OBJETIVO GENERAL

- Estudiar el problema del reconocimiento de las nanocápsulas con contenido de Yodo^{131} radioactivo con la matriz ósea inorgánica de hidroxiapatita.

- Modelar, aplicando supercómputo, el acoplamiento de una nanocápsula de Carbono con Calcio y contenido de Yodo^{131} y el componente mineral cristalino de hidroxipatita [$Ca_{10}(PO_4)_6(OH)_2$] presente en la estructura molecular del hueso.



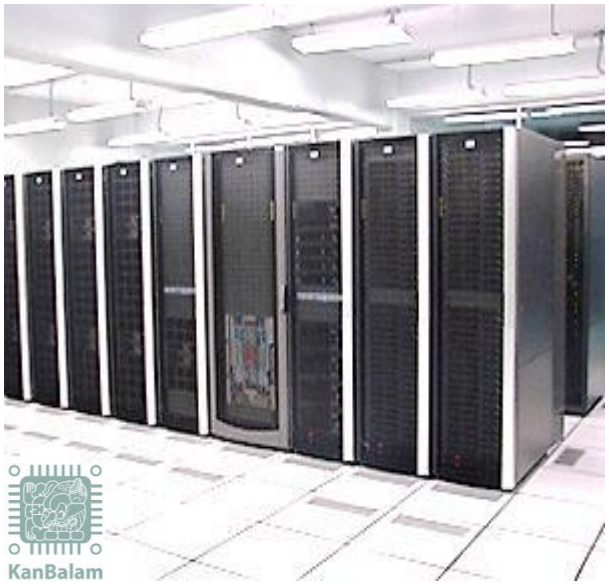
El hueso es el tejido diana de metástasis en el 95% de los pacientes con mieloma múltiple, 75% de los pacientes con cáncer de mama y próstata y un 30-40% en los pacientes con cáncer de pulmón.

Supercómputo para la investigación científica

Supercomputadora KanBalam

Cuando se puso en funcionamiento, en enero de 2007, estaba considerada como la supercomputadora 28 a nivel mundial y la número 1 en América Latina.

- 1,368 procesadores Opteron AMD de 2.6 GHz
- Memoria RAM total de 3 mil gigabytes
- Almacenamiento de 160 terabytes (TB) en 768 discos duros.



Supercomputadora KanBalam, Centro de Supercómputo DGSCA UNAM.

Supercomputadora NES

Nuevo Equipo de Supercómputo 2013 perteneciente al Centro de Supercómputo de la DGSCA UNAM.

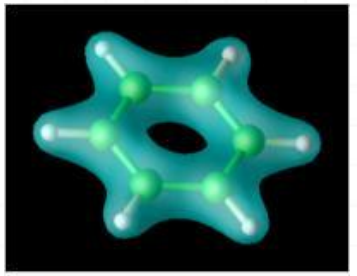
- 250 Nodos regulares: con 2 procesadores Intel Xeon Sandy Bridge E5-2670 a 2.6 GHz con 8 cores cada uno y 32 GB en memoria RAM.
- 8 Nodos GPU: con 2 procesadores Intel Xeon Sandy Bridge E5-2670 a 2.6 GHz con 8 cores cada uno, 32 GB en memoria RAM y 2 unidades de procesamiento gráfico GPU Nvidia TESLA M2090 con 6 GB de memoria (GDDR5).
- 10 Nodos especiales: con 2 procesadores Intel Xeon Sandy Bridge E5-2670 a 2.6 GHz con 8 cores cada uno y 256 GB en memoria RAM.

La supercomputadora más potente de América Latina:

Rank	Name	Site	Country	Vendor	Model	Processor	Nodes	Cores	Rmax(GFlops)	Rpeak
1	MIZTLI	Universidad Nacional Autónoma de México - UNAM	Mexico	Hewlett Packard	HP Cluster Platform 3000SL	Intel E5-2670	332	5280	80429	120500
2	CENAPAD-SP	IBM P750 Centro Nacional Processamento Alto Desempenho - CENAPAD-SP	Brazil	IBM P750	PowerPC_	POWER7	40	1280	27020	37000
3	LEVQUE	National Laboratory for High Performance Computing - NLHPC	Chile	IBM	iDataPlex	Xeon Nehalem X5550	88	528	4847	5639
4	MEDUSA	Centro de Investigaciones en Óptica, A.C. - DO	Mexico	Lufac Computacion S.A. de C.V.	LD-40	Xeon X5675	36	432	4842	5305
5	ISAAC	Comisión Nacional de Energía Atómica CNEA - GTIC/GCAP/GCAP	Argentina	SIASA (INTEL)	Heterogeneo	Xeon X32207/Xeon E5420	182	644	2922	5610
6	Sunhpc	National Laboratory for Scientific Computing - CENAPAD-RJ, UNCC	Brazil	Sun	Sun Blade X6250	Xeon E5440 2830.0	72	568	1681	5293
7	TROQUIL	Centro de	Chile	SGI	Altix UV 2000	Xeon MO-BN	12	96	1547	1843

DFT: Ecuaciones de Kohn y Sham

$$\left\{-\frac{\nabla^2}{2}+\sum_I \frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|}+\int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+v_{xc}(\mathbf{r})\right\}\psi_i(\mathbf{r})=\epsilon_i\psi_i(\mathbf{r})$$



Representación de la densidad electrónica de una molécula de Benceno en el estado fundamental Wikipedia

Pseudopotenciales

$$n(\mathbf{r})=\sum_{\text{ocupados}}|\psi(\mathbf{r})|^2$$

Densidad electrónica

Aproximación de Densidad Local

$$E[n(\mathbf{r})]=T_s[n(\mathbf{r})]+\int v(\mathbf{r})n(\mathbf{r})\,d\mathbf{r}+\frac{1}{2}\iint\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,d\mathbf{r}\,d\mathbf{r}'+E_{xc}[n(\mathbf{r})]$$

Pruebas ADF con enlaces químicos

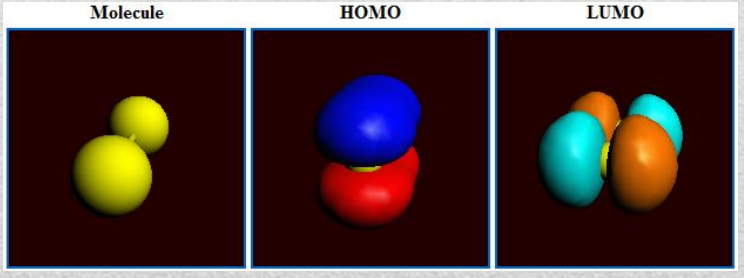
Longitud de Enlace en pm (1×10^{-12} m)

Enlace	CHANG	
H–H	74	74
H–C	109	108
H–N	101	101
H–O	96	96
H–F	92	94
H–Cl	127	129
H–Br	141	144

Enlace	CHANG	
C–H	109	108
C–C	154	154
C=C	134	135
C≡C	120	121
I–H	161	146
I–C	214	210
I–I	267	266

Enlace	CHANG	
O–H	96	96
O–C	143	143
O–O	148	149
O=O	121	121
O=C	121	121

Orbitales Moleculares C-C

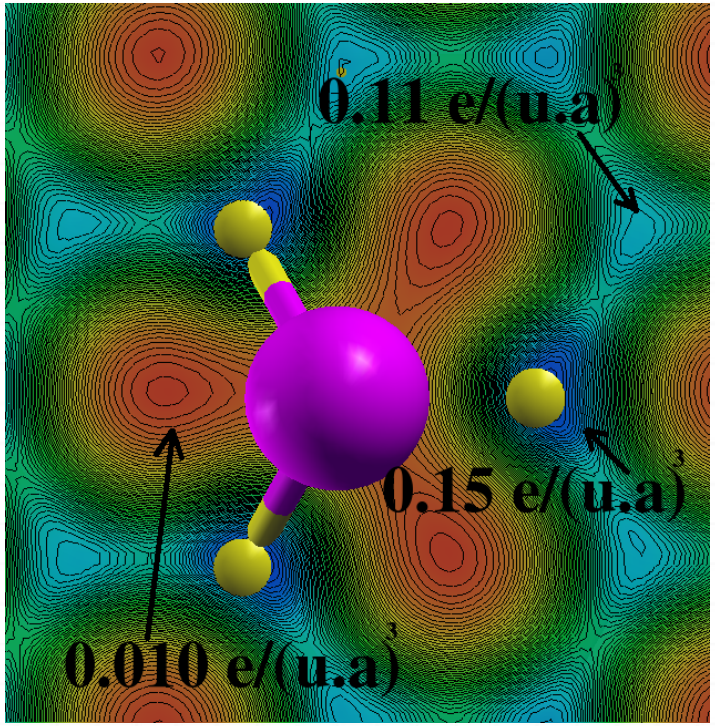


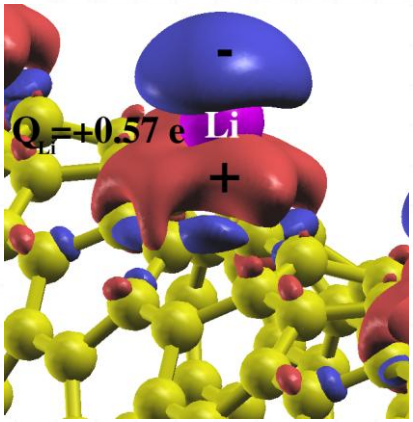
Configuración electrónica del carbono: $[He]2s^2 2p^2$

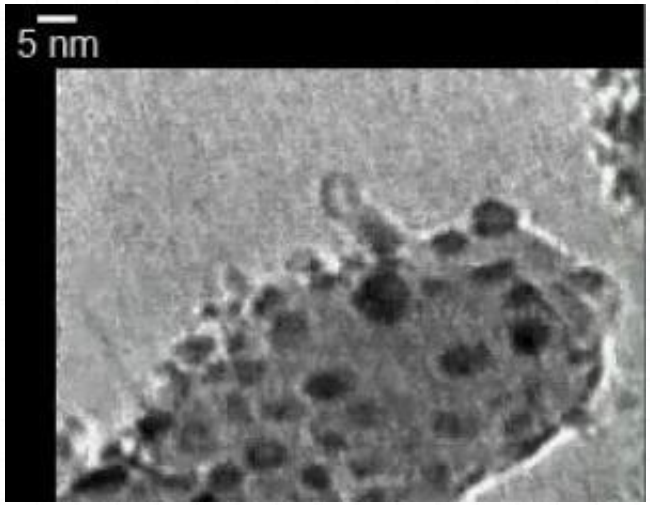
Funcional de Densidad Electrónica

Es posible probar diferentes propiedades moleculares usando la:

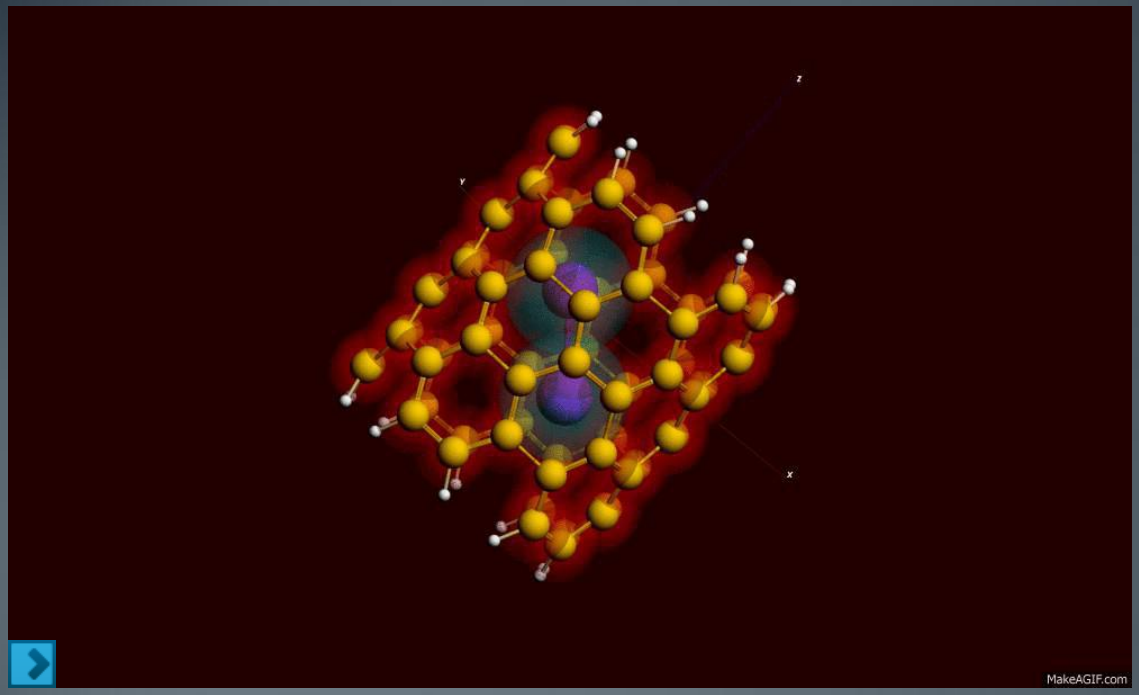
TEORÍA DE LA FUNCIONAL DE DENSIDAD ELECTRÓNICA



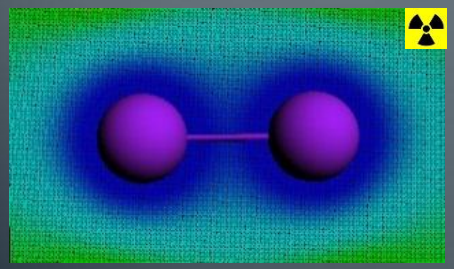




Interacción de un Nanotubo $C_{90}H_{20}$ con $^{131}I_2$

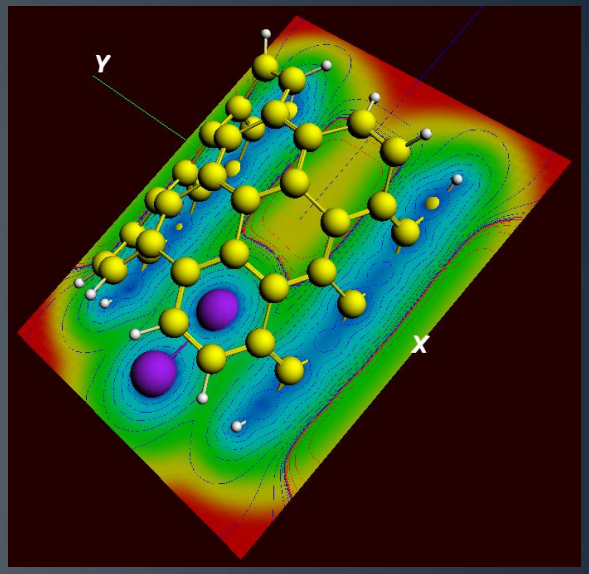


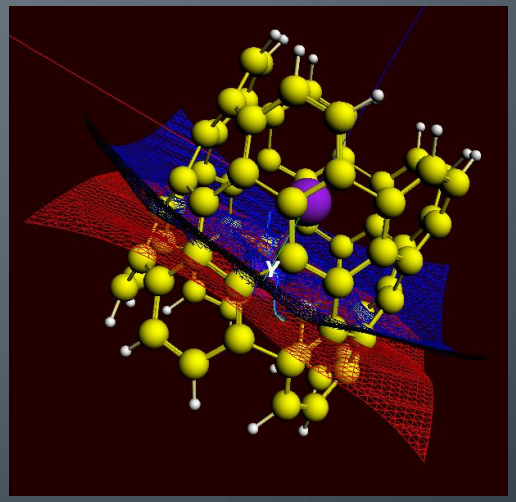
Optimización Geométrica



Potencial Eléctrico del $^{131}I_2$

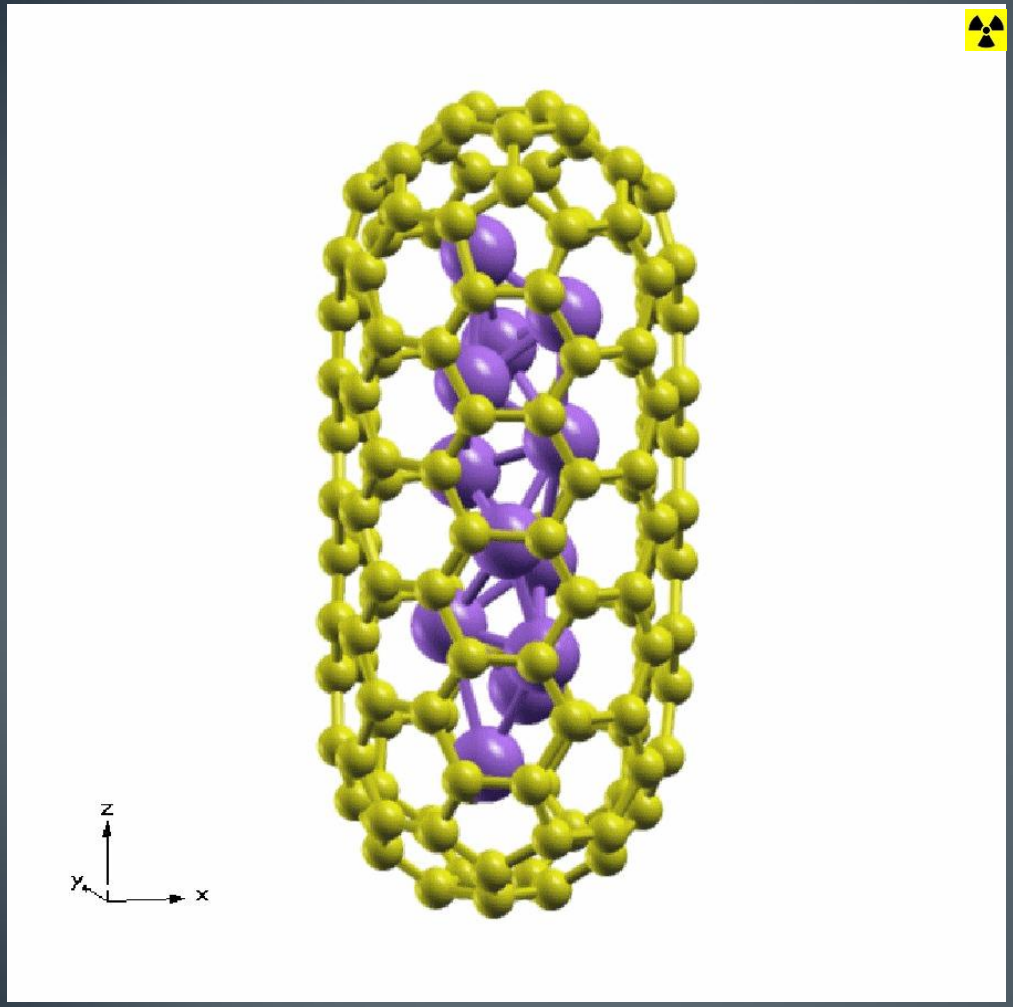
Mapa de Potencial Eléctrico

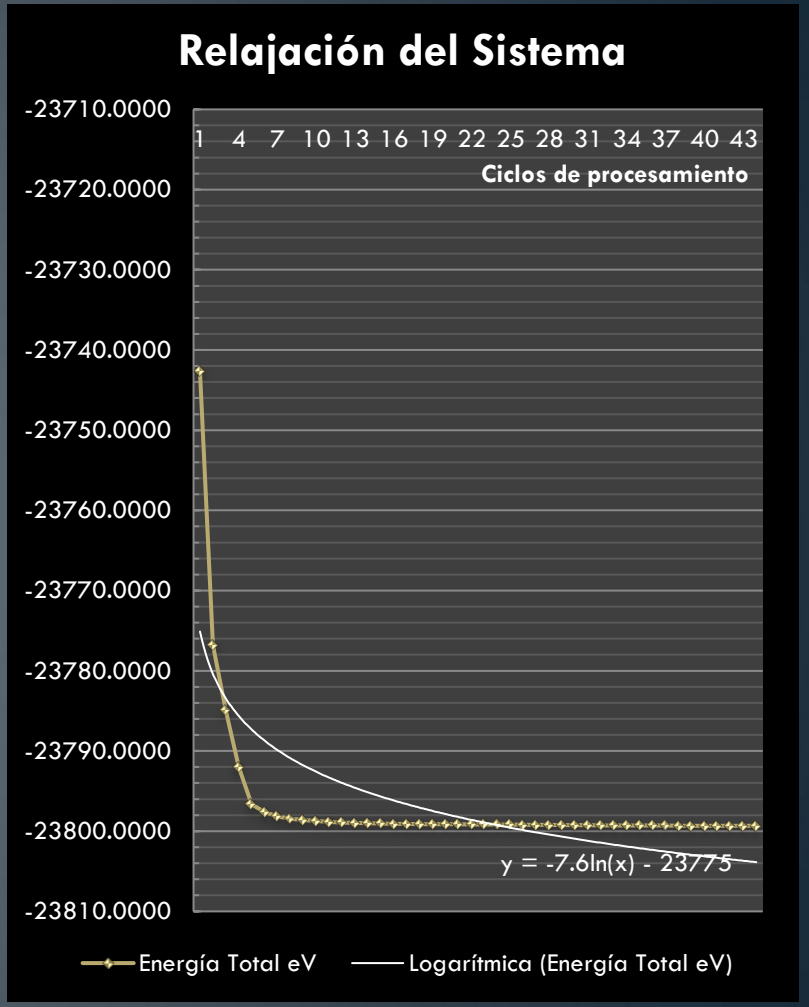




El campo eléctrico molecular del nanotubo de carbono repele a la molécula de Yodo

Relajación NC_{130} con 6 $^{131}I_2$





Energía Total del Estado Base = -23,799.3247 eV

atomic species	valence	mass	pseudopotential
C	4.00	12.0000	C (1.00)
I	7.00	132.0900	I (1.00)

32 MPs, AMD 2 GHz
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X-window CRYstalline Structures and DENsities

B) Pentaceno

Científicos del centro de investigación de IBM en Zúrich junto al microscopio de fuerzas atómicas.- IBM

Los átomos que forman una molécula se han logrado visualizar bien a través de un Microscopio de Fuerzas Atómicas (AFM) del Laboratorio IBM en Zúrich (Suiza) .

La molécula es el pentaceno ($C_{22}H_{14}$), consistente en cinco anillos de benceno enlazados formando una cadena aromática.

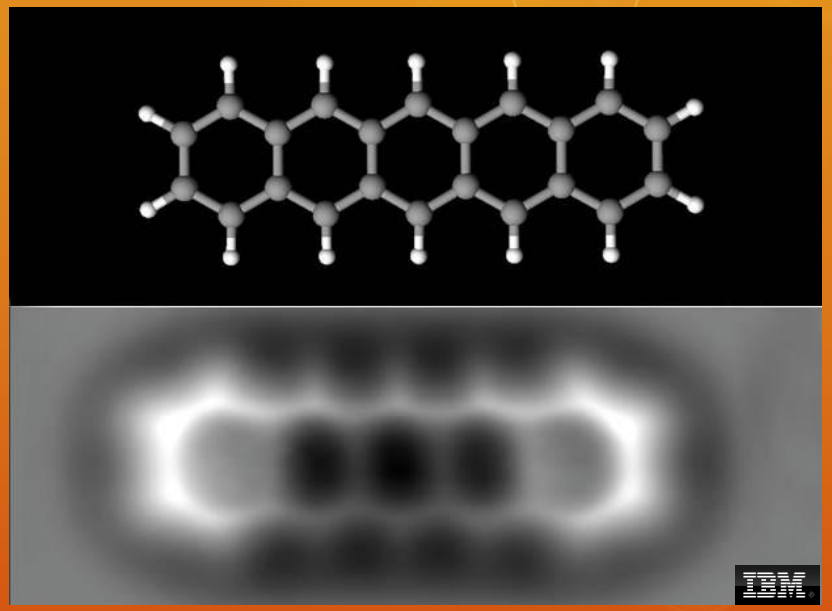
Esto se ha publicado en la revista *Science*,

En otro experimento, publicado en la misma revista, el equipo midió los estados de carga de los átomos con el mismo tipo de microscopio. Así se podrá investigar cómo se trasmite la carga a través de las moléculas o de redes moleculares.

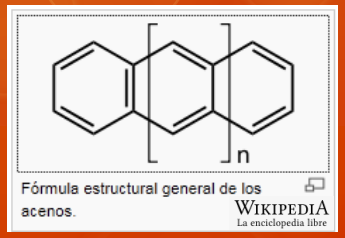
Además, los investigadores han conseguido descubrir que la fuerza repulsiva que les ha permitido obtener el contraste suficiente para la imagen procede del efecto cuántico denominado principio de exclusión de Pauli.

En los últimos años, se había conseguido definir nano estructuras a escala atómica y ahora ha sido posible mostrar la estructura química de una molécula con una resolución atómica, viendo los átomos individuales.

Según Gerhard Meyer se puede considerar este hecho similar a la capacidad de traspasar un tejido blando con rayos X para obtener una imagen nítida de los huesos.



Estructura interna de una molécula de pentaceno, de 1,4 nanómetros de longitud. Abajo, modelo de la misma (los átomos grises son de carbono y los blancos de hidrógeno).- IBM

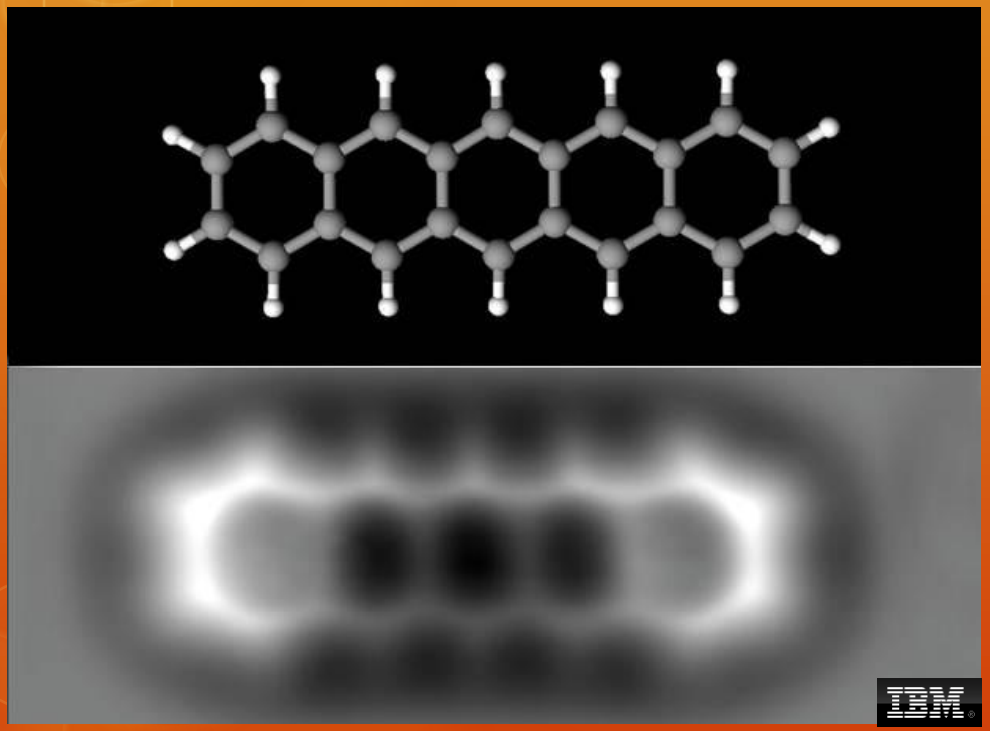


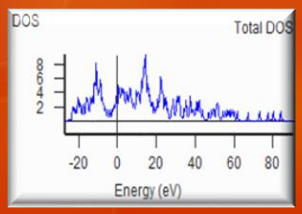
Fórmula estructural general de los acenos.

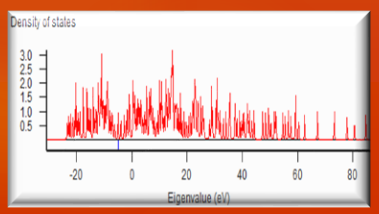
WIKIPEDIA
La enciclopedia libre

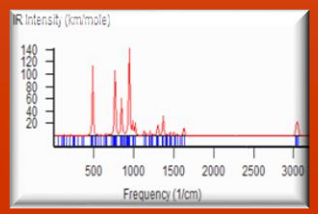
ADF Mapas de potencial eléctrico en $C_{22}H_{14}$

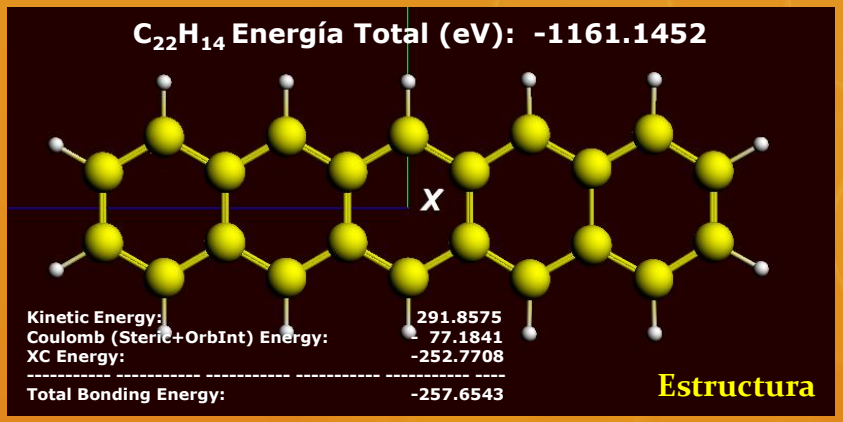
Estructura interna de una molécula de pentaceno, de 1.4 nanómetros de longitud. (los átomos grises son de carbono y los blancos de hidrógeno).- IBM

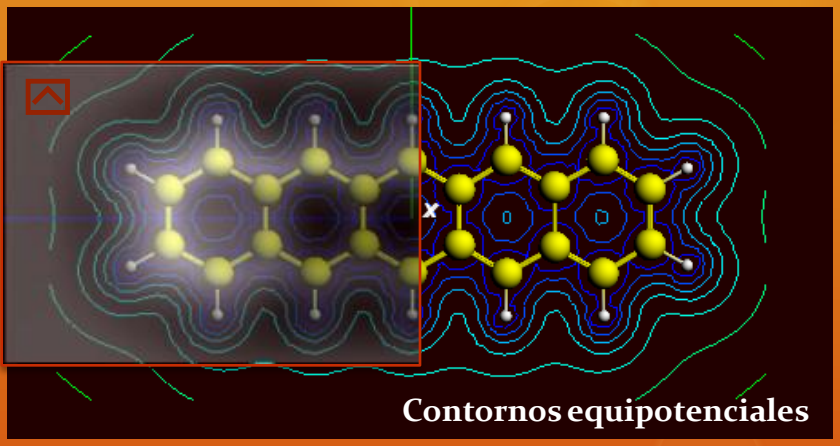


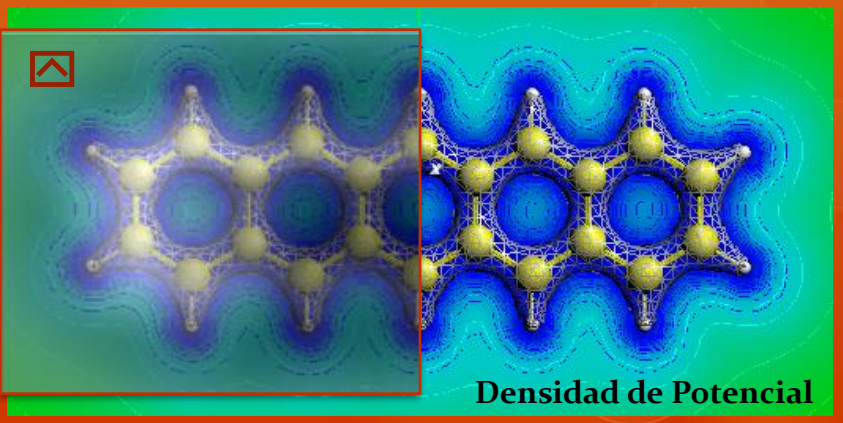








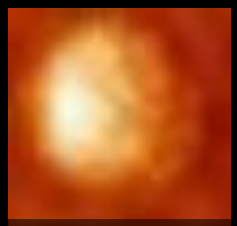




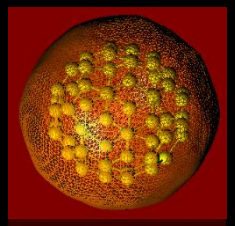
Fulereno C_{60}

Buckminsterfullerene

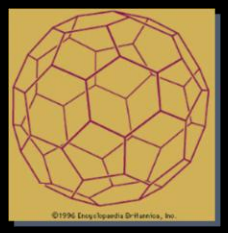
$E_0 = E_c + E_p = -9{,}304.80$ eV



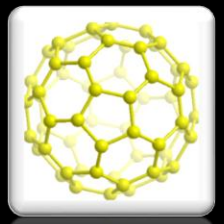
Microscopio de Efecto Túnel, STM

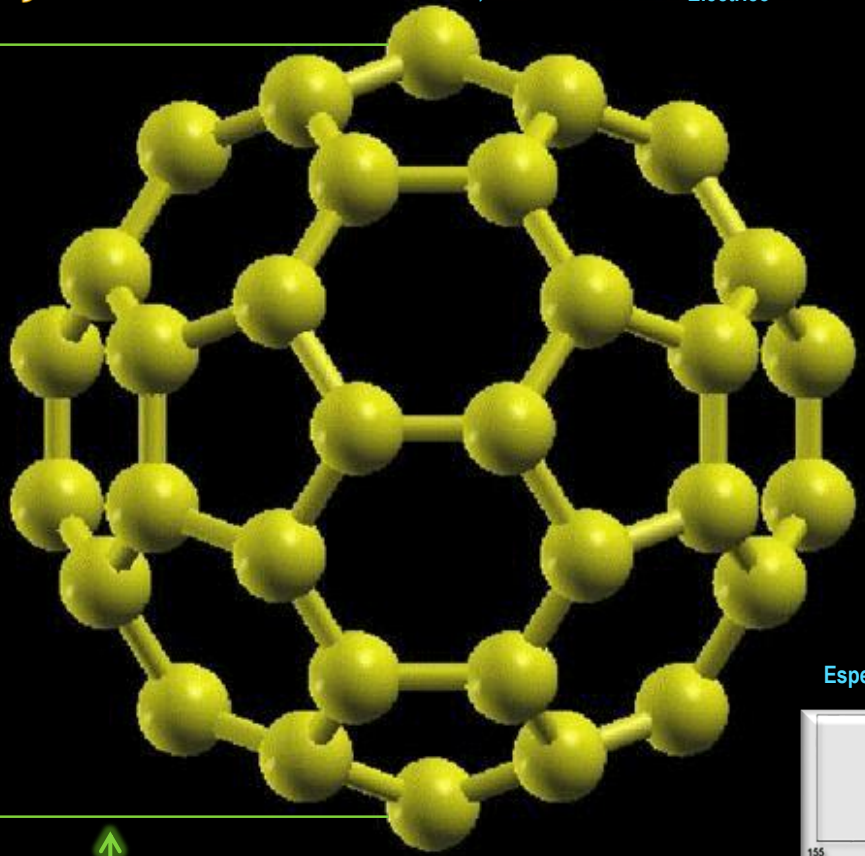


Superficie de Potencial Eléctrico

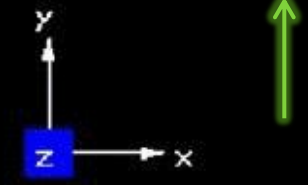


Icosaedro Truncado



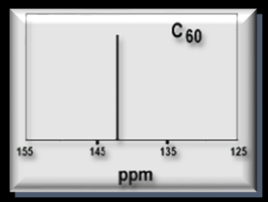


$D(C_{60}) = 6.78$ Å



$\langle d(C\text{-}C) \rangle = 1.436$ Å

Espectroscopia RMN



Carbono, C6 (12 uma)
Configuración Electrónica : $[He]2s^2 2p^2$

C	1	0	3,449997	0,6848
C	2	3,002716	1,408493	-1,170975
C	3	0	-3,449997	0,6848
C	4	2,279007	-2,579483	-0,723694
C	5	-2,579483	-0,723694	2,279007
C	6	-1,170975	-3,002716	1,408493
C	7	-1,170975	3,002716	1,408493
C	8	-2,579483	0,723694	2,279007
C	9	2,279007	2,579483	-0,723694
C	10	3,002716	-1,408493	-1,170975
C	11	-3,002716	-1,408493	-1,170975
C	12	-3,002716	1,408493	-1,170975
C	13	-0,723694	2,279007	-2,579483
C	14	0,6848	0	-3,449997
C	15	-0,723694	-2,279007	-2,579483
C	16	-2,279007	2,579483	-0,723694
C	17	0,723694	2,279007	-2,579483
C	18	1,408493	-1,170975	-3,002716
C	19	-1,170975	-3,002716	-1,408493
C	20	-3,449997	-0,6848	0
C	21	2,579483	0,723694	2,279007
C	22	2,579483	-0,723694	2,279007
C	23	1,408493	-1,170975	3,002716
C	24	0,6848	0	3,449997
C	25	1,408493	1,170975	3,002716
C	26	1,170975	3,002716	1,408493
C	27	3,449997	0,6848	0
C	28	2,279007	-2,579483	0,723694
C	29	-0,723694	-2,279007	2,579483
C	30	-1,408493	1,170975	3,002716
C	31	1,170975	-3,002716	1,408493
C	32	-1,408493	-1,170975	3,002716
C	33	-0,723694	2,279007	2,579483
C	34	2,279007	2,579483	0,723694
C	35	3,449997	-0,6848	0
C	36	-2,279007	-2,579483	-0,723694
C	37	-3,449997	0,6848	0
C	38	-1,170975	3,002716	-1,408493
C	39	1,408493	1,170975	-3,002716
C	40	0,723694	-2,279007	-2,579483
C	41	-0,6848	0	-3,449997
C	42	-1,408493	-1,170975	-3,002716
C	43	-2,579483	-0,723694	-2,279007
C	44	-2,579483	0,723694	-2,279007
C	45	-1,408493	1,170975	-3,002716
C	46	1,170975	3,002716	-1,408493
C	47	2,579483	-0,723694	-2,279007
C	48	0	-3,449997	-0,6848
C	49	-3,002716	-1,408493	1,170975
C	50	-2,279007	2,579483	0,723694
C	51	-0,6848	0	3,449997
C	52	0,723694	2,279007	2,579483
C	53	3,002716	1,408493	1,170975
C	54	3,002716	-1,408493	1,170975
C	55	0,723694	-2,279007	2,579483
C	56	-2,279007	-2,579483	0,723694
C	57	-3,002716	1,408493	1,170975
C	58	0	3,449997	-0,6848
C	59	2,579483	0,723694	-2,279007
C	60	1,170975	-3,002716	-1,408493

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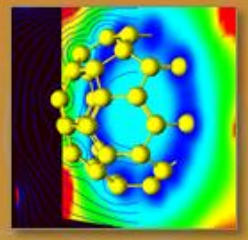
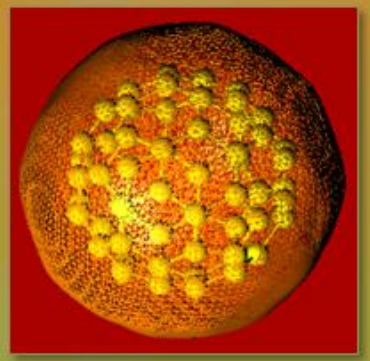
Generation of Nano-Geometries
SCH

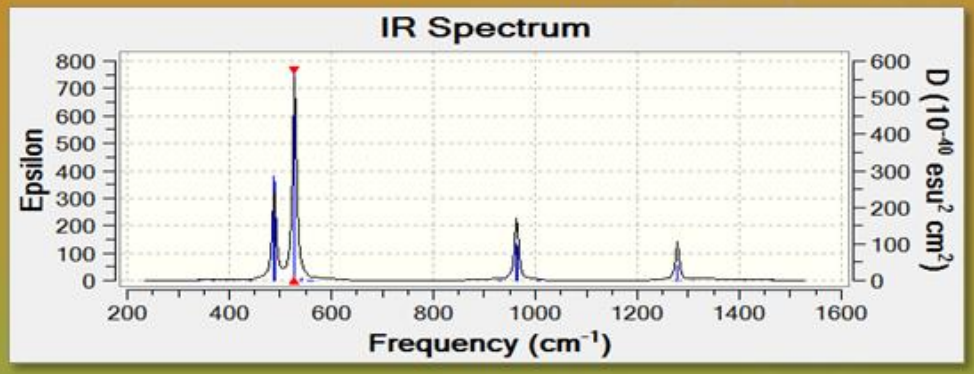
El Fullereno C_{60}



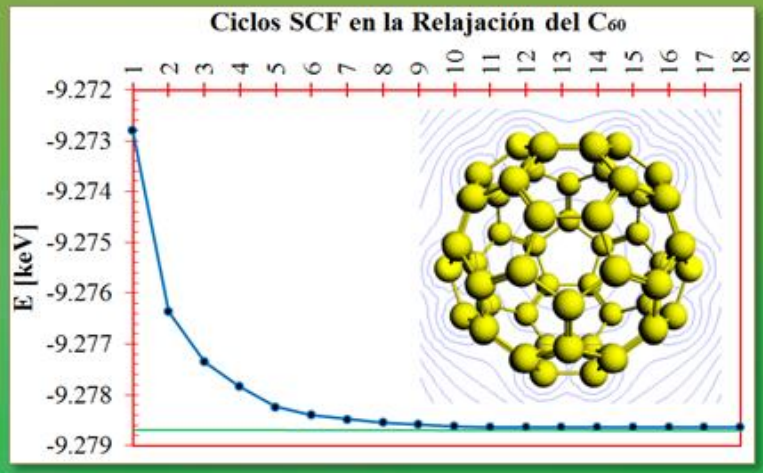


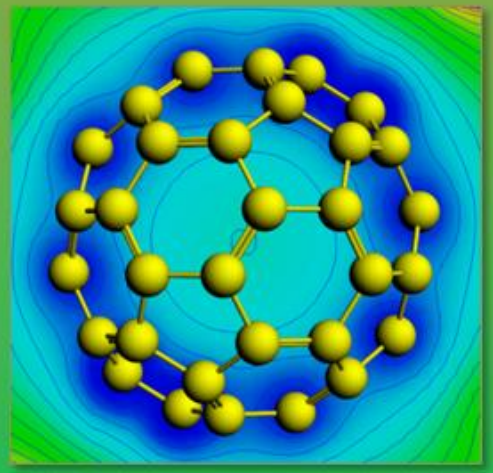
Simulación de la Superficie de Potencial Eléctrico.

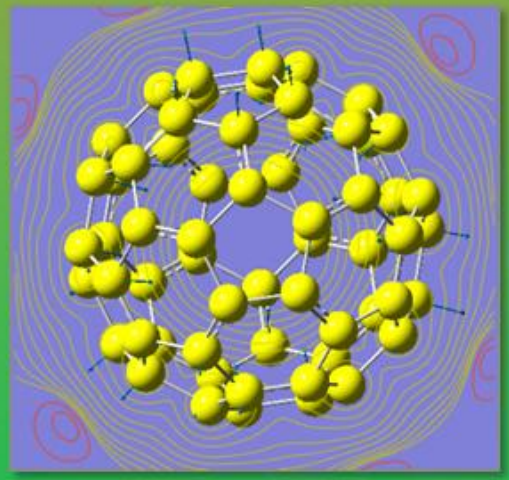
Vista del C_{60} con el Microscopio de Efecto Túnel.



Espectro infra rojo (IR) obtenido mediante una simulación con el software Gaussian para el cálculo de la estructura electrónica molecular del fullereno C_{60}.







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intel Inside CORE i3
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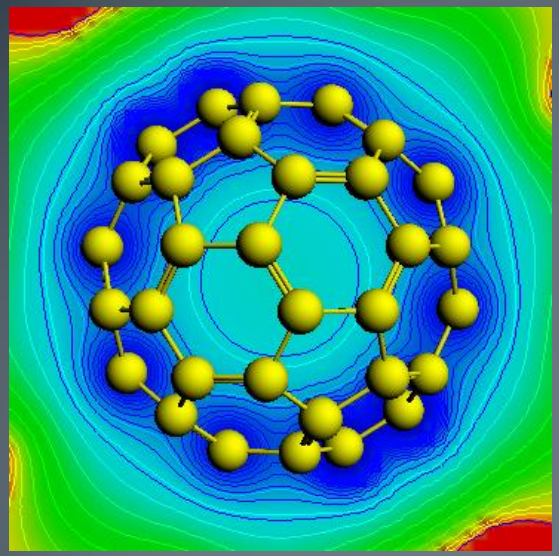
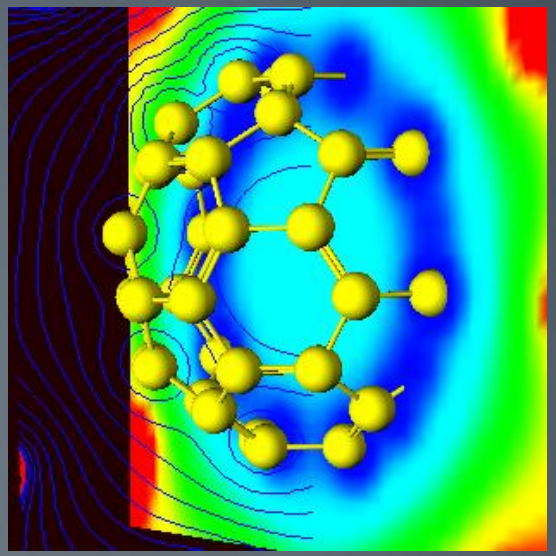
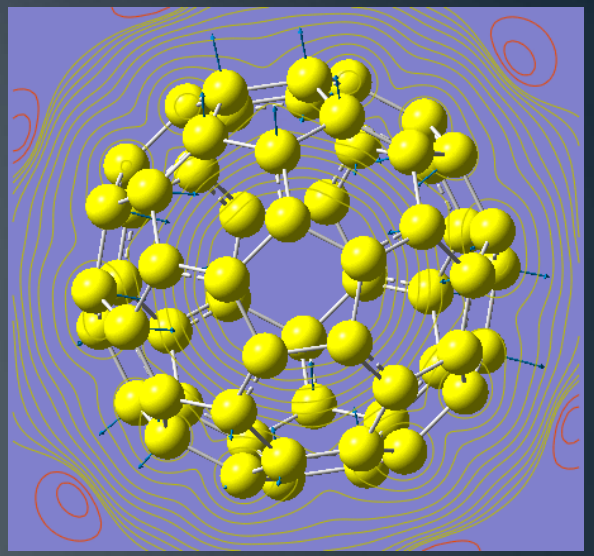
Potencial Eléctrico y Vibraciones del C_{60}





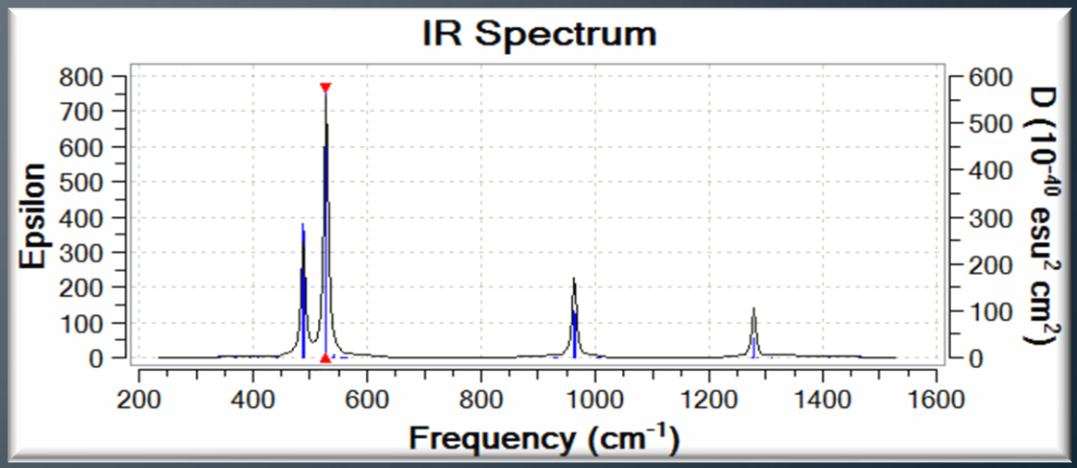


Energía de Enlace LDA - 554.1522 eV
Energía Total SP -2,780.5846 eV
Total XC: -7,715.2889 eV

XC = Intercambio y Correlación LDA

Principales Frecuencias de Oscilación IR

Frecuencia Principal (cm^{-1}) = 528.98 <Exp*>
4 Bandas Activas en el Espectro IR
174 modos de vibración



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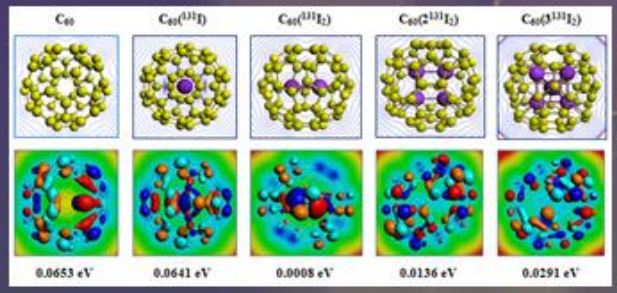
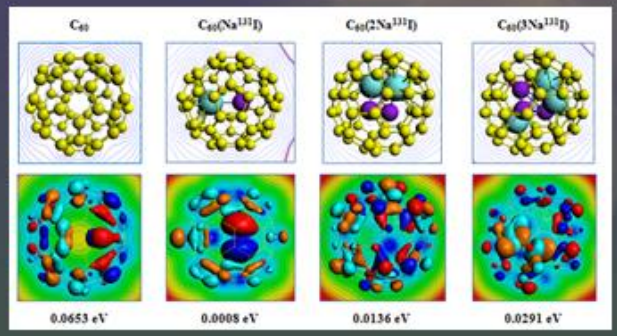
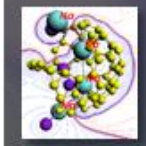
Lista de Algunos Resultados

OPTIMIZACIONES GEOMÉTRICAS Y DINÁMICAS MOLECULARES







1. Relajación del fullereno C_{60}
2. Relajación del fullereno $C_{60}(3^{131}I_2)$
3. Buckyball con adsorción de calcio, C_{60} + 13 Ca
4. Buckyball con adsorción de fósforo, C_{60} + 13 P
5. Interacción del fullereno $C_{60}(3^{131}I_2)$ con calcio
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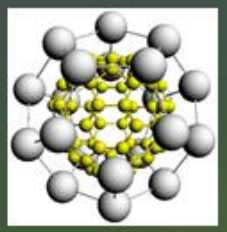
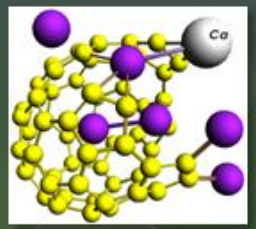
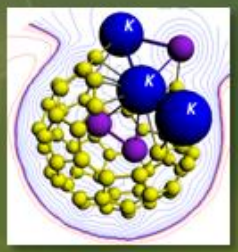
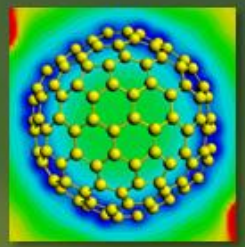
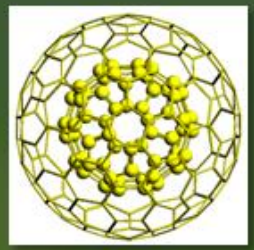
7. Relajación del fullereno C_{180}
8. Nanocápsula multicapa $C_{180}(C_{60})$
9. Nanocápsula multicapa con contenido radioactivo, $C_{180}(C_{60}(3^{131}I_2))$
10. Interacción de calcio (Ca) con la Nanocápsula multicapa $C_{180}(C_{60}(3^{131}I_2))$
11. Interacción de la Nanocápsula multicapa $C_{180}(C_{60}(3^{131}I_2))$ + 20Ca con una molécula de hidroxiapatita (HA)

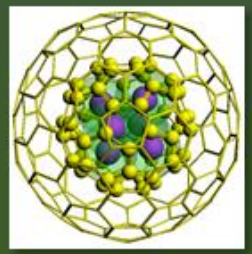


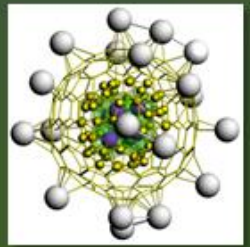


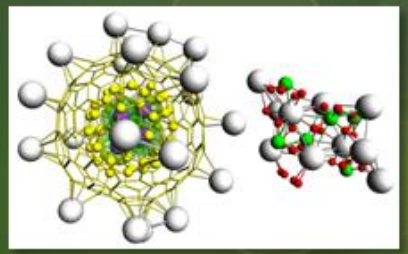












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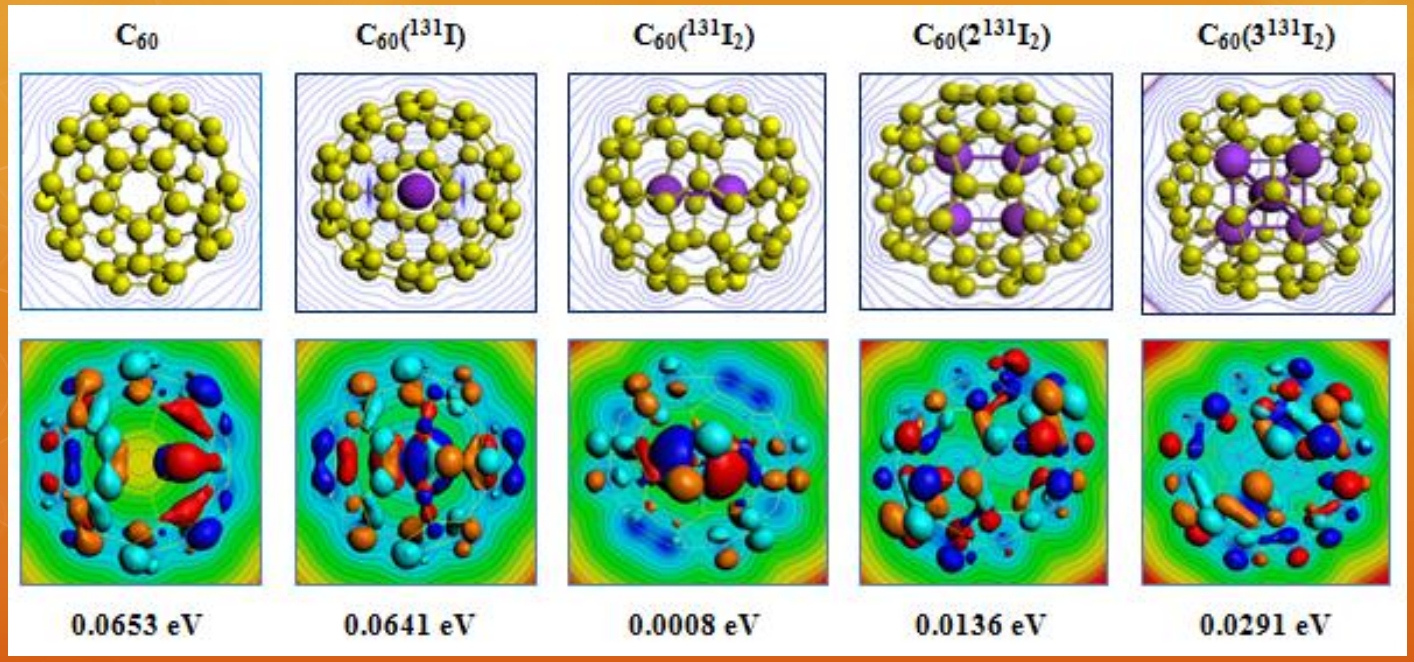

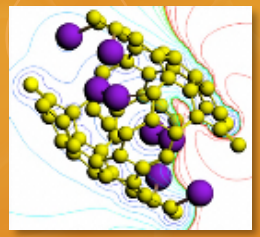

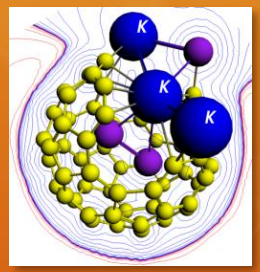

1. **Relajación del fullereno C_{60}.**
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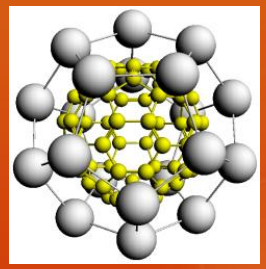

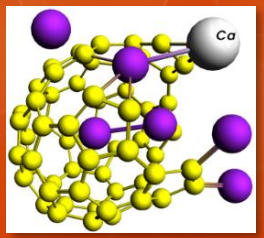

INTERNATIONAL CONFERENCE ON DIAMOND AND CARBON MATERIALS 2013
2-5 SEPTEMBER 2013
Riva del Garda
ITALY

[P2.076]
Encapsulating radioactive iodine ^{131}I in C_{60}

A. Valderrama[1,2], J. Guzmán[1], L.F. Magaña*[2]

[1]Instituto Politécnico Nacional, México, [2]Universidad Nacional Autónoma de México, México

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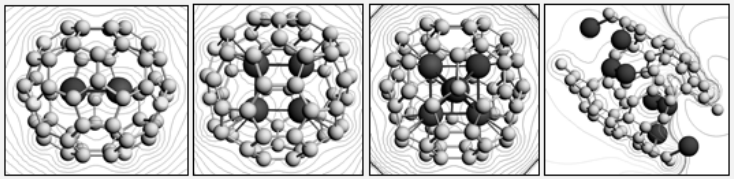
Presenter Index

Magaña, L.F.
Universidad Nacional Autónoma de México, México

Encapsulating radioactive iodine ^{131}I in C_{60}

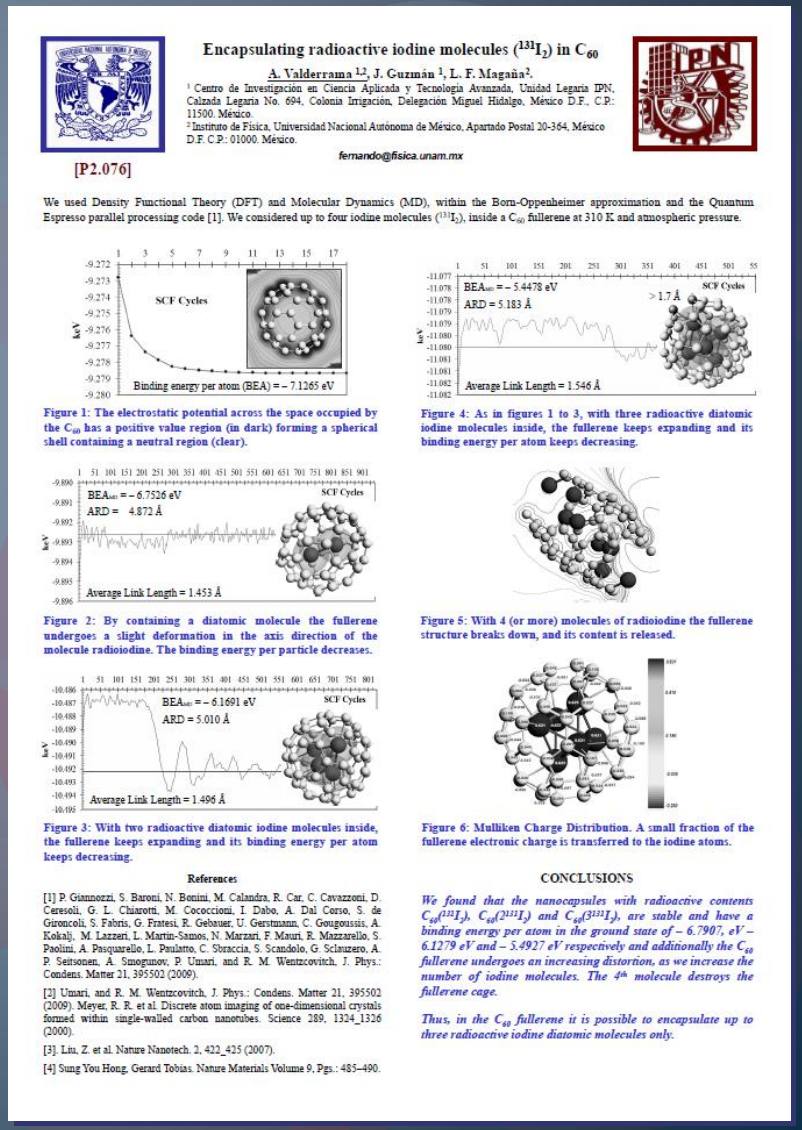
Wednesday, 4 September 2013: Session 20: Poster 2 and refreshments - 17:00-18:00

We used density functional theory and molecular dynamics, within the Born-Oppenheimer approximation and the Quantum Espresso code [1]. We considered up to four iodine molecules ($^{131}I_2$), inside a C_{60} fullerene at 300 K. and atmospheric pressure. We found that the C_{60} capsule undergoes an increasing distortion, as we increase the number of iodine molecules. The 4th molecule destroys the fullerene cage. Thus, in the C_{60} fullerene it is possible to encapsulate up to three radioactive iodine diatomic molecules only. Below we show the final configurations of the molecular dynamics at 300 K and atmospheric pressure, for one, two, three, and four encapsulated molecules, respectively.



$C_{60}(\mathbf{1}^{131}I_2)$ $C_{60}(\mathbf{2}^{131}I_2)$ $C_{60}(\mathbf{3}^{131}I_2)$ $C_{60}(\mathbf{4}^{131}I_2)$

[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto,C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P.
[2] Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395502 (2009).
Meyer, R. R. et al. Discrete atom imaging of one-dimensional crystals formed within single-walled carbon nanotubes. Science 289, 1324_1326 (2000).
[3]. Liu, Z. et al. Nature Nanotech. 2, 422_425 (2007).
[4] Sung You Hong, Gerard Tobias. Nature Materials Volume: 9, Pages: 485–490



Encapsulating radioactive iodine molecules ($^{131}I_2$) in C_{60}

A. Valderrama [1,2], J. Guzmán [1], L. F. Magaña [2].
[1] Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada, Unidad Legaria IPN, Calzada Legaria No. 694, Colonia Irrigación, Delegación Miguel Hidalgo, México D.F., C.P.: 11500. México.
[2] Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, México D.F. C.P.: 01000. México.
fernando@fisica.unam.mx

[P2.076]

We used Density Functional Theory (DFT) and Molecular Dynamics (MD), within the Born-Oppenheimer approximation and the Quantum Espresso parallel processing code [1]. We considered up to four iodine molecules ($^{131}I_2$), inside a C_{60} fullerene at 310 K and atmospheric pressure.

Figure 1: The electrostatic potential across the space occupied by the C_{60} has a positive value region (in dark) forming a spherical shell containing a neutral region (clear).

Figure 4: As in figures 1 to 3, with three radioactive diatomic iodine molecules inside, the fullerene keeps expanding and its binding energy per atom keeps decreasing.

Figure 2: By containing a diatomic molecule the fullerene undergoes a slight deformation in the axis direction of the molecule radioiodine. The binding energy per particle decreases.

Figure 5: With 4 (or more) molecules of radioiodine the fullerene structure breaks down, and its content is released.

Figure 3: With two radioactive diatomic iodine molecules inside, the fullerene keeps expanding and its binding energy per atom keeps decreasing.

Figure 6: Mulliken Charge Distribution. A small fraction of the fullerene electronic charge is transferred to the iodine atoms.

References

[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395502 (2009).

[2] Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395502 (2009). Meyer, R. R. et al. Discrete atom imaging of one-dimensional crystals formed within single-walled carbon nanotubes. Science 289, 1324_1326 (2000).

[3]. Liu, Z. et al. Nature Nanotech. 2, 422_425 (2007).

[4] Sung You Hong, Gerard Tobias. Nature Materials Volume 9, Pgs.: 485–490.

CONCLUSIONS

We found that the nanocapsules with radioactive contents $C_{60}(^{131}I_2)$, $C_{60}(^{2131}I_2)$ and $C_{60}(^{3131}I_2)$, are stable and have a binding energy per atom in the ground state of – 6.7907, eV – 6.1279 eV and – 5.4927 eV respectively and additionally the C_{60} fullerene undergoes an increasing distortion, as we increase the number of iodine molecules. The 4th molecule destroys the fullerene cage.

Thus, in the C_{60} fullerene it is possible to encapsulate up to three radioactive iodine diatomic molecules only.

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Journal of Molecular Modeling

Encapsulation of sodium radio-iodide in fullerene C60

--Manuscript Draft--

Manuscript Number:	JMMO-D-13-00499R1
Full Title:	Encapsulation of sodium radio-iodide in fullerene C60
Article Type:	Original paper
Keywords:	Fullerene, buckyball, C60, nanocapsule, sodium radio-iodide.
Corresponding Author:	Alejandro Valderrama, Master in Science (Physics) CICATA-Legaria, IPN Ciudad de México, D. F. MEXICO
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Order of Authors:	Alejandro Valderrama, Master in Science (Physics)
	José Guzmán, PhD
Order of Authors Secondary Information:	
Abstract:	In this work we have studied the well-known "Buckminsterfullerene" C60 containing different amounts, from one to four molecules, of sodium radio-iodide (Na131I), with Density Functional Theory geometrical optimizations and molecular dynamics at 310 K and atmospheric pressure. We found that nanocapsules with the radioactive content Na131I@C60, 2Na131I@C60 and 3Na131I@C60 are stable. Furthermore, the C60 fullerene undergoes expansion when the number of sodium radio-iodide molecules inside increases. Utilizing the Mulliken charge distribution analysis it was shown that a small charge transfer occurs from iodine to fullerene's carbon atoms. This produces repulsion which increases bond lengths thus the structure is weakened while the binding energy per atom decreases. For the case in which the fullerene initially contains four sodium radio-iodide molecules the expansion is greater than that which the structure can withstand. So the fullerene breaks and releases its contents. This result leads us to conclude that the fullerene can encapsulate up to 3 molecules of sodium radio-iodide.
Response to Reviewers:	Response to reviewers letter is attached.

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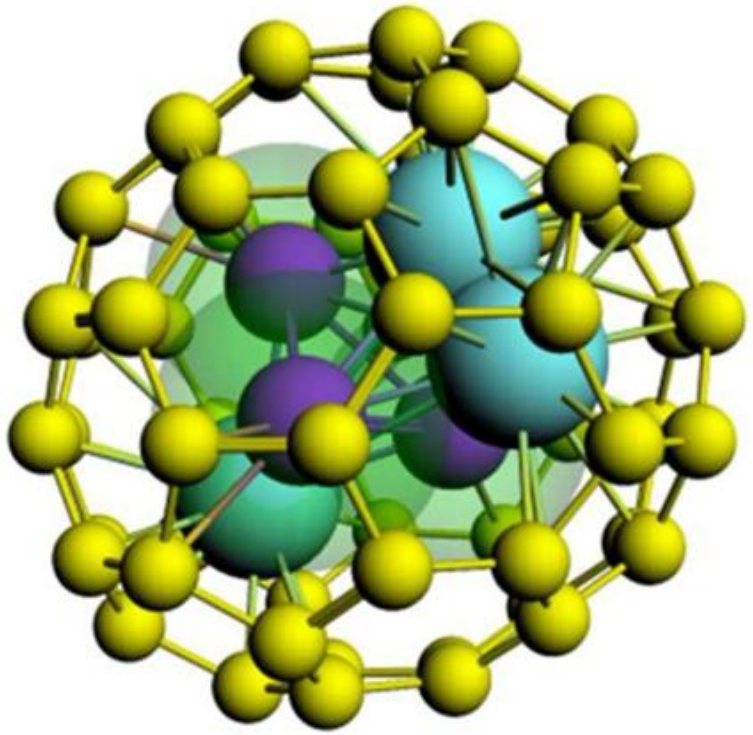

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Encapsulation of sodium radio-iodide in fullerene C_{60}

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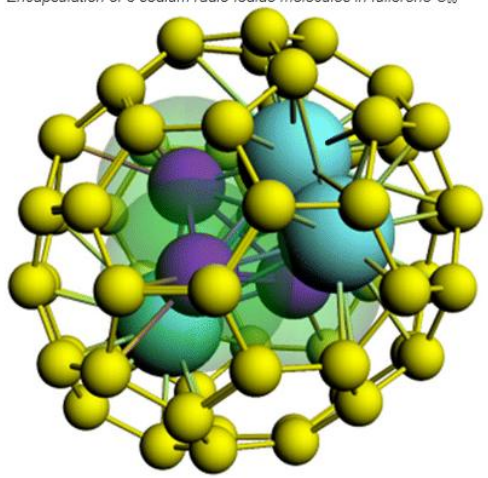
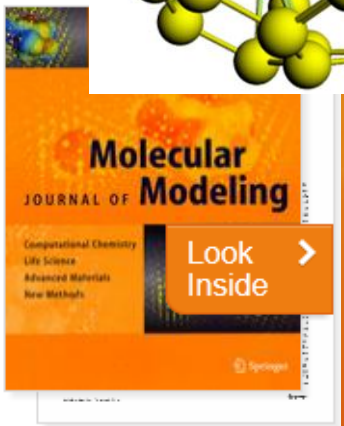
Abstract

In this work we have studied the well-known "Buckminsterfullerene" C_{60} containing different amounts, from one to four molecules, of sodium radio-iodide ($Na^{131}I$), with density functional theory geometrical optimizations and molecular dynamics at 310 K and atmospheric pressure. We found that nanocapsules with the radioactive content $Na^{131}I@C_{60}$, $2Na^{131}I@C_{60}$ and $3Na^{131}I@C_{60}$ are stable.

Figure
Encapsulation of 3 sodium radio-iodide molecules in fullerene C_{60}





Within this Article

- Introduction
- Methods
- Results and discussion
- Conclusions
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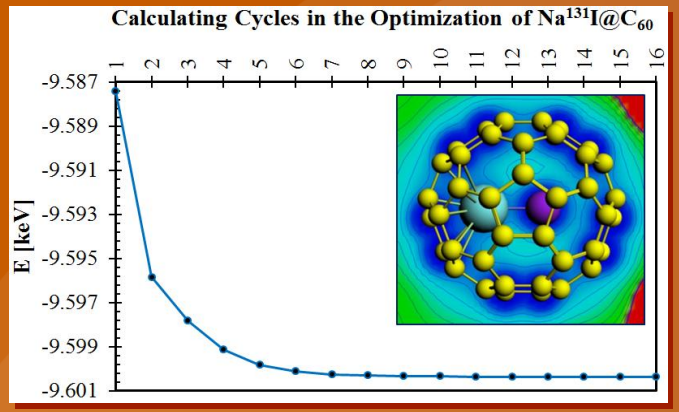
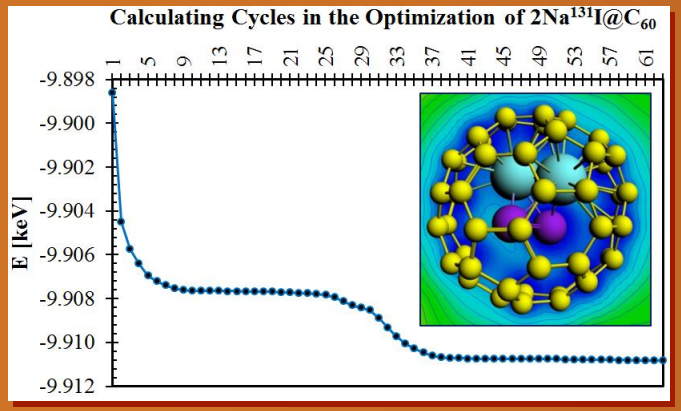
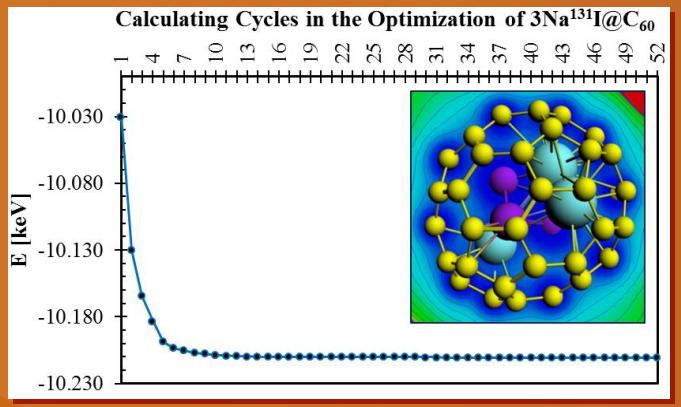
Resultados Presentados en el Artículo







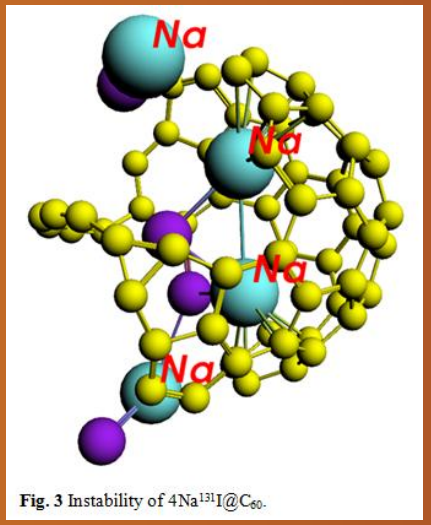
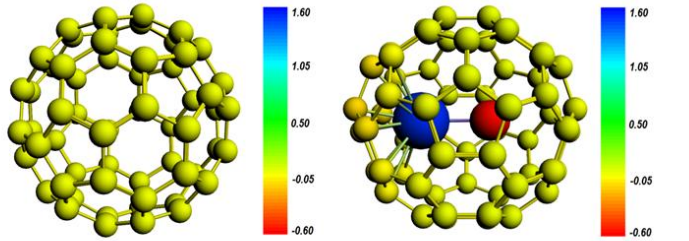


Fig. 3 Instability of $4Na^{131}I@C_{60}$.

Con 4 moléculas de $Na^{131}I@C_{60}$ el fullereno se rompe

Mulliken electronic charge distributions

We have obtained the empty C_{60} molecule's Mulliken electronegativity and, with one to three sodium radio-iodide molecules inside. Initially empty C_{60} is practically neutral, as the sodium radio-iodide content rises, a "slight" shift of negative charges occurs from the iodine ^{131}I atoms toward the buckyball's carbon atoms, see Fig. 4. This produces some repulsion of the carbon atoms so explains that their binding energy diminishes, bonds become longer, and the structure is weakened.



Análisis Electrónico

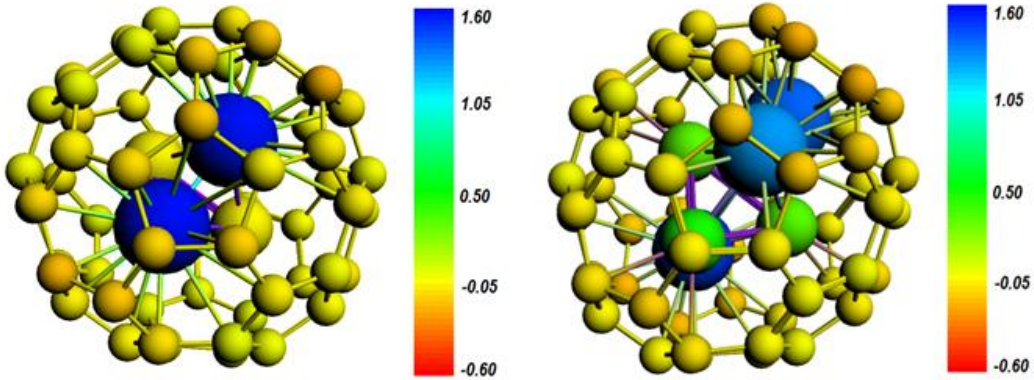
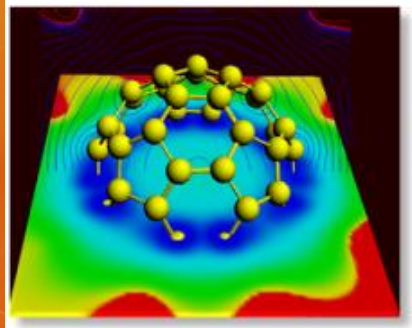


Fig. 4 Charge distribution trend on the Mulliken scale of the empty C_{60} and with one to three $Na^{131}I$ molecules inside.

Interacción del Fullereno con contenido radioactivo con Ca, P y Sr

[F 1] Fullereno C_{60}

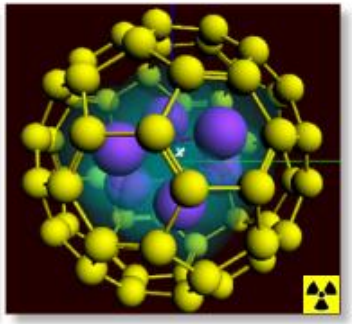
Arreglo esférico. Los átomos ocupan los vértices de 20 hexágonos y 12 pentágonos ninguno de los cuales comparte un borde con otro **TBE = -9,304.80 eV**



[F 2] BuckyBall con contenido de Yodo

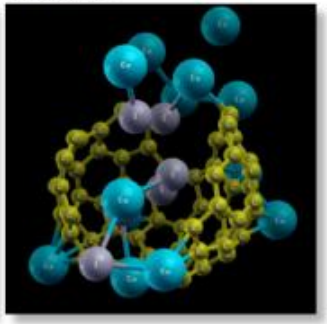
Se simularon 3 moléculas de yodo radioactivo en el interior

Total Bond Energy LDA
-394.1065 eV



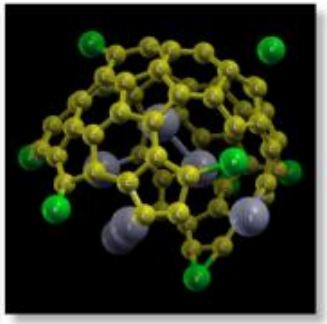
[F 3] Nanocápsula en un gas de Ca

El gas de calcio en principio fue adsorbido superficie pero terminó por romper la nano estructura liberando su contenido.



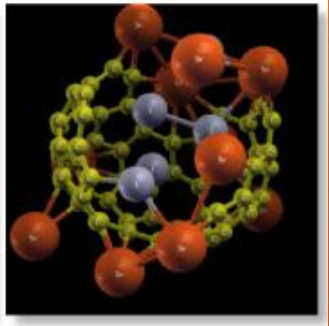
[F 4] Nanocápsula en un gas de P

El sustrato de silicio se simuló con la estructura cristalina del diamante



[F 5] Nanocápsula en un gas de Sr

El sustrato de silicio se simuló con la estructura cristalina del diamante



ACEPTACIÓN EN CONGRESOS INTERNACIONALES

$C_{180}(C_{60})$ MULTILAYER NANOCAPSULE CONTAINING RADIOACTIVE IODINE $3^{131}I_2$

ENCAPSULATION RADIOIODINE LIMIT IN THE FULLERENE C60 AND INTERACTIONS OF THESE NANOCAPSULES WITH CALCIUM ATOMS

INTERNATIONAL CONFERENCE ON DIAMOND AND CARBON MATERIALS 2013

2-5 SEPTEMBER 2013
Riva del Garda
ITALY

[P2.076]
Encapsulating radioactive iodine ^{131}I in C_{60}

A. Valderrama[1,2], J. Guzmán[1], L.F. Magaña*[2]

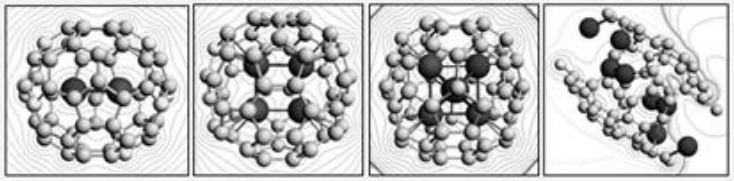
[1]Instituto Politécnico Nacional, México, [2]Universidad Nacional Autónoma de México, México

Programme | Titles | Presenters | Topics

Presenter Index

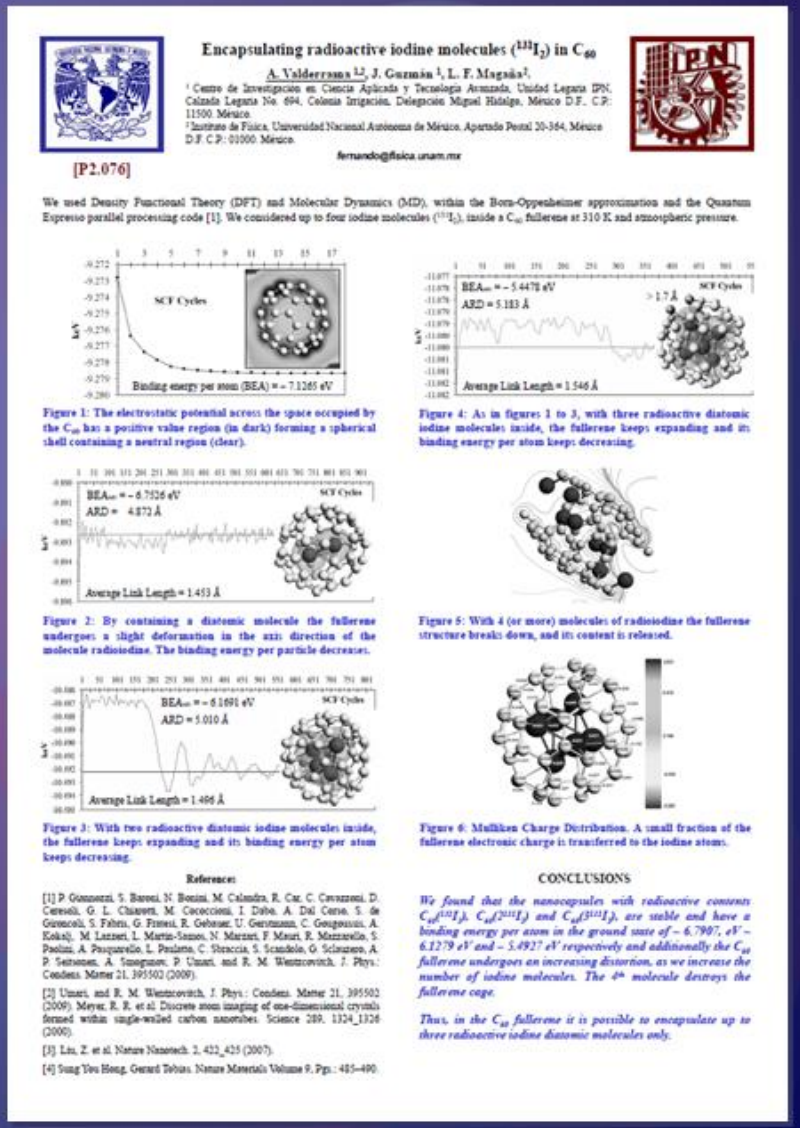
Magaña, L.F.
Universidad Nacional Autónoma de México, México
Encapsulating radioactive iodine ^{131}I in C_{60}
Wednesday, 4 September 2013, Session 20: Poster 2 and refreshments - 17:00-18:00

We used density functional theory and molecular dynamics, within the Born-Oppenheimer approximation and the Quantum Espresso code [1]. We considered up to four iodine molecules ($^{131}I_2$), inside a C_{60} fullerene at 300 K. and atmospheric pressure. We found that the C_{60} capsule undergoes an increasing distortion, as we increase the number of iodine molecules. The 4th molecule destroys the fullerene cage. Thus, in the C_{60} fullerene it is possible to encapsulate up to three radioactive iodine diatomic molecules only. Below we show the final configurations of the molecular dynamics at 300 K and atmospheric pressure, for one, two, three, and four encapsulated molecules, respectively.



$C_{60}(1^{131}I_2)$ $C_{60}(2^{131}I_2)$ $C_{60}(3^{131}I_2)$ $C_{60}(4^{131}I_2)$

[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto,C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P.
[2] Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395502 (2009).
Meyer, R. R. et al. Discrete atom imaging of one-dimensional crystals formed within single-walled carbon nanotubes. Science 289, 1324_1326 (2000).
[3]. Liu, Z. et al. Nature Nanotech. 2, 422_425 (2007).
[4] Sung You Hong, Gerard Tobias. Nature Materials Volume: 9, Pages: 485–490



Encapsulating radioactive iodine molecules ($^{131}I_2$) in C_{60}

A. Valderrama [1,2], J. Guzmán [1], L. F. Magaña [2].
[1] Centro de Investigación en Ciencia Aplicada y Tecnología Avanzada, Unidad Legaria IPN. Calzada Legaria No. 694, Colonia Irrigación, Delegación Miguel Hidalgo, México D.F., C.P. 11500. México.
[2] Instituto de Física, Universidad Nacional Autónoma de México. Apartado Postal 20-364, México D.F. C.P.: 01000. México.
fernando@fisica.unam.mx

[P2.076]

We used Density Functional Theory (DFT) and Molecular Dynamics (MD), within the Born-Oppenheimer approximation and the Quantum Espresso parallel processing code [1]. We considered up to four iodine molecules ($^{131}I_2$), inside a C_{60} fullerene at 310 K and atmospheric pressure.

Figure 1: The electrostatic potential across the space occupied by the C_{60} has a positive value region (in dark) forming a spherical shell containing a neutral region (clear).

Figure 4: As in figures 1 to 3, with three radioactive diatomic iodine molecules inside, the fullerene keeps expanding and its binding energy per atom keeps decreasing.

Figure 2: By containing a diatomic molecule the fullerene undergoes a slight deformation in the axis direction of the molecule radioiodine. The binding energy per particle decreases.

Figure 5: With 4 (or more) molecules of radioiodine the fullerene structure breaks down, and its content is released.

Figure 3: With two radioactive diatomic iodine molecules inside, the fullerene keeps expanding and its binding energy per atom keeps decreasing.

Figure 6: Mulliken Charge Distribution. A small fraction of the fullerene electronic charge is transferred to the iodine atoms.

References

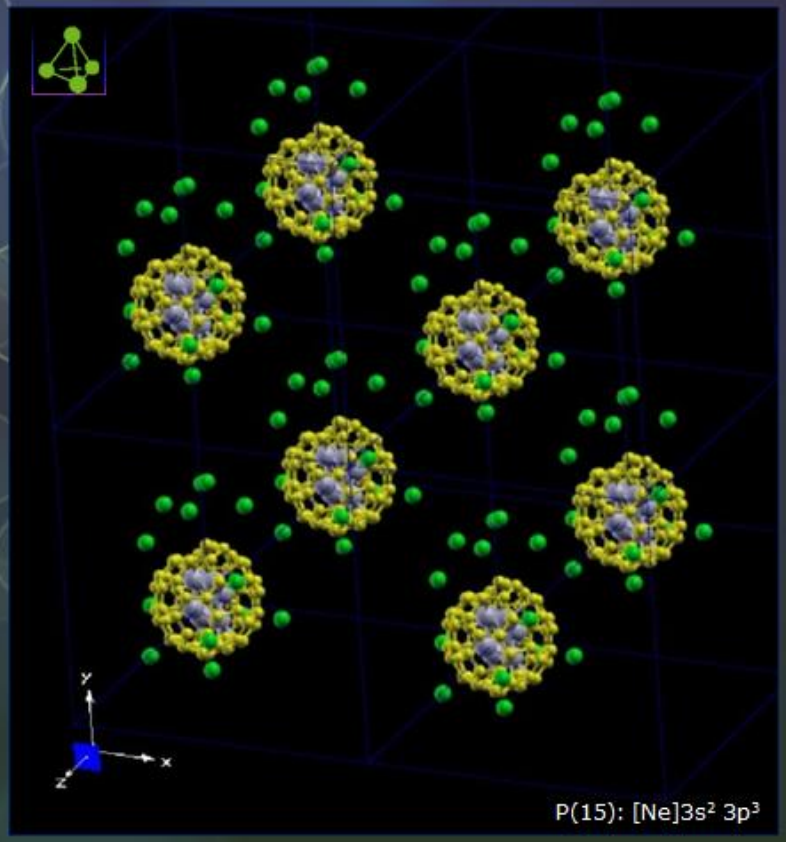
[1] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395502 (2009).
[2] Umari, and R. M. Wentzcovitch, J. Phys.: Condens. Matter 21, 395502 (2009). Meyer, R. R. et al. Discrete atom imaging of one-dimensional crystals formed within single-walled carbon nanotubes. Science 289, 1324_1326 (2000).
[3] Liu, Z. et al. Nature Nanotech. 2, 422_425 (2007).
[4] Sung You Hong, Gerard Tobias. Nature Materials Volume 9, Pgs.: 485–490.

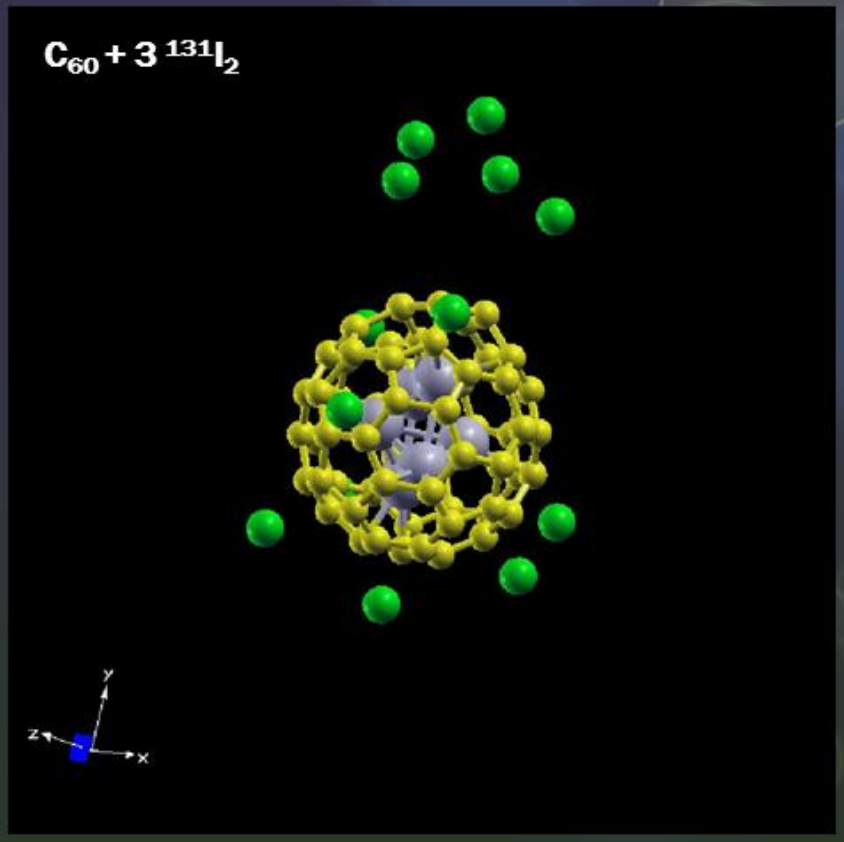
CONCLUSIONS

We found that the nanocapsules with radioactive contents $C_{60}(1^{131}I_2)$, $C_{60}(2^{131}I_2)$ and $C_{60}(3^{131}I_2)$, are stable and have a binding energy per atom in the ground state of – 6.7907, eV' – 6.1279 eV' and – 5.4927 eV' respectively and additionally the C_{60} fullerene undergoes an increasing distortion, as we increase the number of iodine molecules. The 4th molecule destroys the fullerene cage.

Thus, in the C_{60} fullerene it is possible to encapsulate up to three radioactive iodine diatomic molecules only.

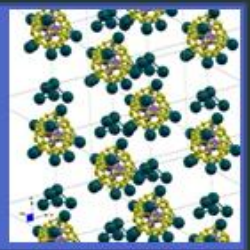
Nanocápsula $C_{60}+3^{131}I_2$ inmersa en Gas de Fósforo^{32}





Nanocápsula $C_{60} + 3^{131}I_2$ inmersa en Gas de Estroncio^{89}

CÁLCULO EN PROCESO



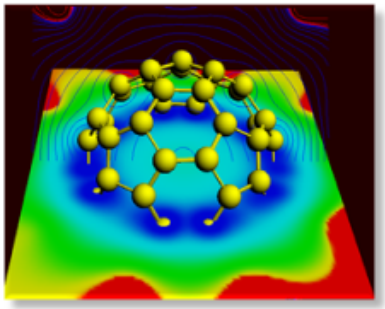
El Fósforo en gas, primero se adhiere a la Nanocápsula de C_{60} para luego romper los enlaces entre los carbonos y con ello la estructura esférica, el contenido de Yodo radioactivo es liberado al medio exterior de la nanocápsula.

KanBalam
COMPUTO academico UNAM
QUANTUM ESPRESSO
AMD Athlon X2
XCrySDen ... X-window CRYstalline Structures and DENsities
intel inside CORE i3
SCH

En el presente trabajo hemos simulado, aplicando supercómputo y, utilizando el código para procesamiento en paralelo Quantum Espresso y la Teoría de Funcional de Densidad Electrónica (DFT) en su Aproximación de Densidad Local (LDA) utilizando el pseudopotencial de conservación de norma Perdew-Burke-Erzerhof (PBE) exch-corr, el conocido Buckminster fullerene C_{60} [F 1] conteniendo 3 moléculas diatómicas de yodo radioactivo ($3^{131}I_2$) [F 2]. Este sistema presentó inestabilidad en presencia de átomos de calcio, Ca [F 3], fósforo, P [F 4] y estroncio, Sr [F 5], los cuales al ser adsorbidos en su superficie, rompieron el fullereno liberando su contenido de yodo radioactivo.

[F 1] Fullereno C_{60}

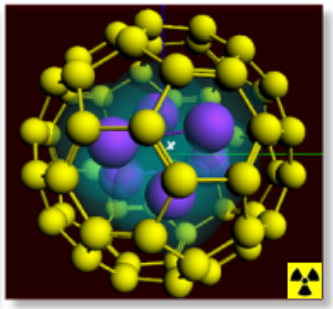
Arreglo esférico. Los átomos ocupan los vértices de 20 hexágonos y 12 pentágonos ninguno de los cuales comparte un borde con otro **TBE = -9,304.80 eV**



[F 2] BuckyBall con contenido de Yodo

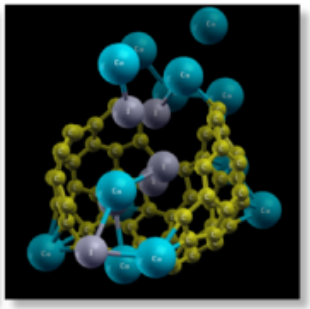
Se simularon 3 moléculas de yodo radioactivo en el interior

Total Bond Energy LDA
-394.1065 eV



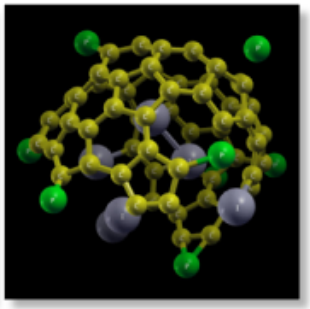
[F 3] Nanocápsula en un gas de Ca

El gas de calcio en principio fue adsorbido superficie pero terminó por romper la nano estructura liberando su contenido.



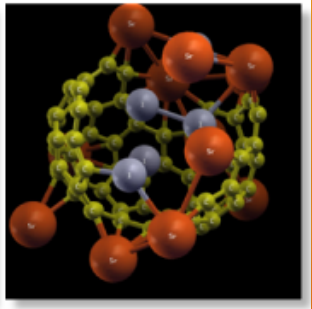
[F 4] Nanocápsula en un gas de P

El sustrato de silicio se simuló con la estructura cristalina del diamante



[F 5] Nanocápsula en un gas de Sr

El sustrato de silicio se simuló con la estructura cristalina del diamante

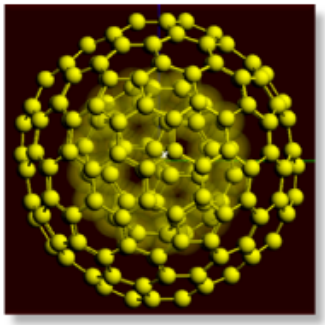


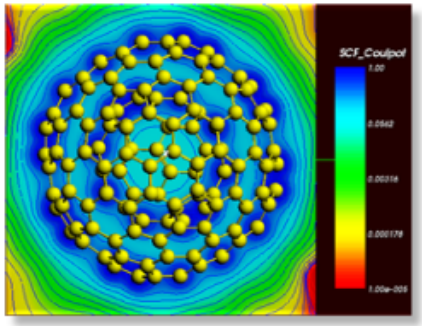
De modo que se realizó la simulación del fullereno multi capa compuesto por el C_{60} contenido en el buckyball C_{180} [F 6]. Encontramos que este nano sistema de dos esferas de carbono concéntricas tiene una energía en el estado base de -37.133 KeV. Este sistema permite almacenar, en la esfera interior C_{60}, 3 moléculas diatómicas de yodo radioactivo ($3^{131}I_2$) [F 7] con una energía para el estado base de – 38.956 KeV y fisisorber en la superficie de la esfera exterior, C_{180}, 10 átomos de calcio con una energía total para el estado base de -49.117 KeV [F8]. El sistema así conformado: $C_{180}(C_{60}(3I_2))$ + 10Ca, es estable y constituye una nano cápsula con contenido radioactivo capaz de interaccionar con otras moléculas con afinidad química con él calcio, como la de fosfato de calcio cristalino $[Ca_{10}(PO_4)6(OH)_2]$ presente en los huesos en forma de hidroxiapatita [F9].

[F 6] Fullereno $C_{180}(C_{60})$

Para este arreglo de dos fullerenos concéntricos se encontró una energía total de relajación para el estado base de: **-2,729.23819 Ry = -37.133 KeV**. Debe observarse que el sistema se encuentra fuertemente ligado.

240 ÁTOMOS, 1440 ELECTRONES

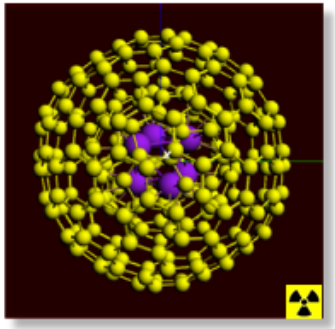


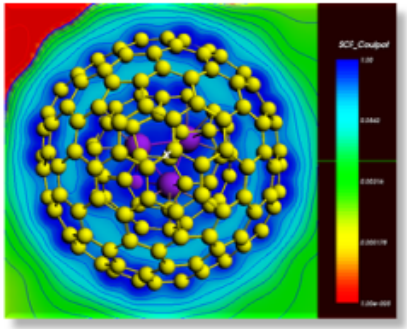


[F 7] Multi nanocápsula $C_{180}(C_{60}) + 3^{131}I_2$

La nanocápsula multicapa con contenido radioactivo presentó una menor energía total del estado base: **-2,863.25052 Ry = -38.956 KeV**. Aun con el contenido de Yodo radioactivo el sistema se mantiene fuertemente ligado.

246 ÁTOMOS, 1748 ELECTRONES





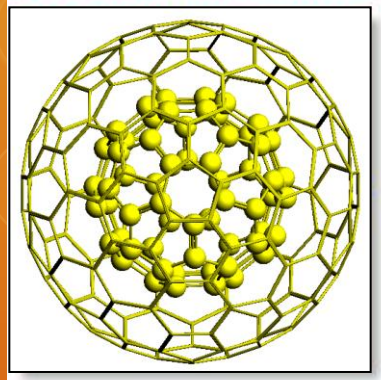
Nanocápsula Multicapa $C_{60}@C_{180}$

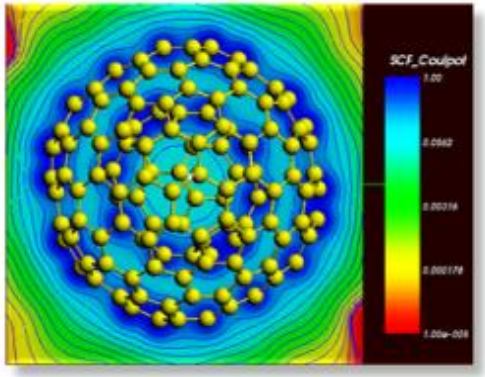
Nanocápsula Multicapa $3I_2@C_{60}@C_{180}$

[F 6] Fullereno $C_{180}(C_{60})$

Para este arreglo de dos fullerenos concéntricos se encontró una energía total de relajación para el estado base de: **-2,729.23819 Ry = -37.133 KeV**.
Debe observarse que el sistema se encuentra fuertemente ligado.

240 ÁTOMOS, 1440 ELECTRONES

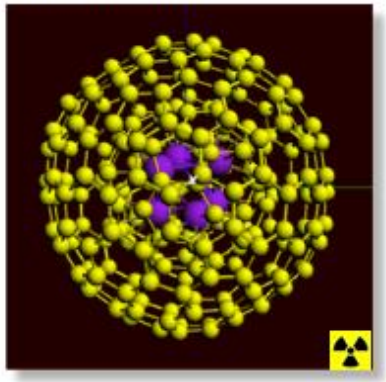


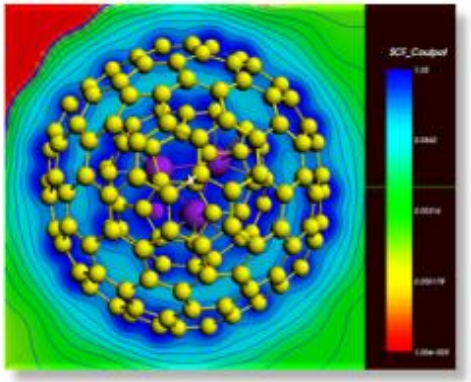


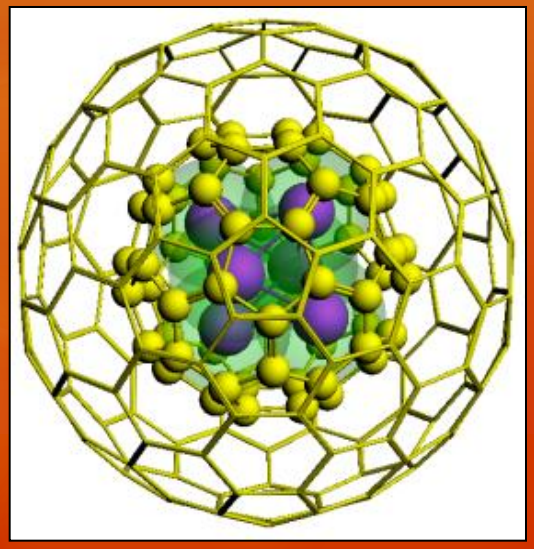
[F 7] Multi nanocápsula $C_{180}(C_{60}) + 3^{131}I_2$

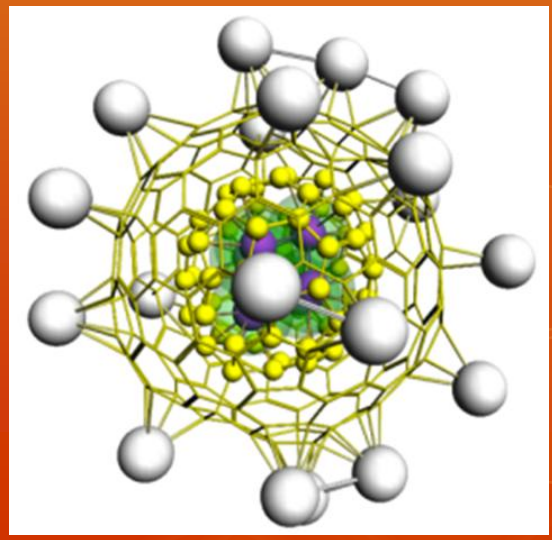
La nanocápsula multicapa con contenido radioactivo presentó una menor energía total del estado base: **-2,863.25052 Ry = -38.956 KeV**.
Aun con el contenido de Yodo radioactivo el sistema se mantiene fuertemente ligado.

246 ÁTOMOS, 1748 ELECTRONES

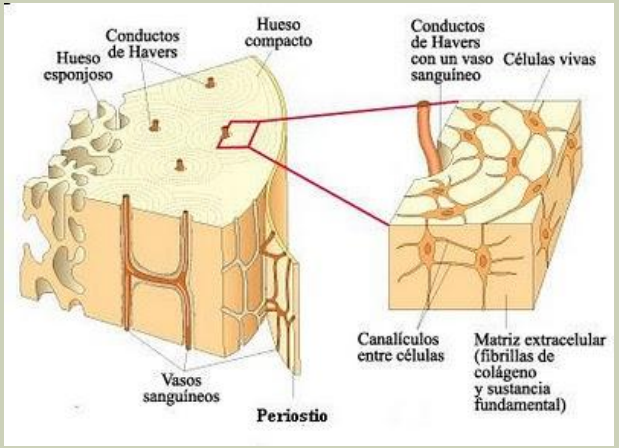




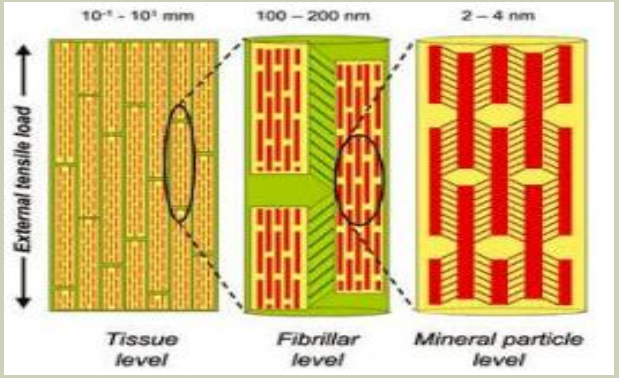




ESTRUCTURA MOLECULAR DEL HUESO

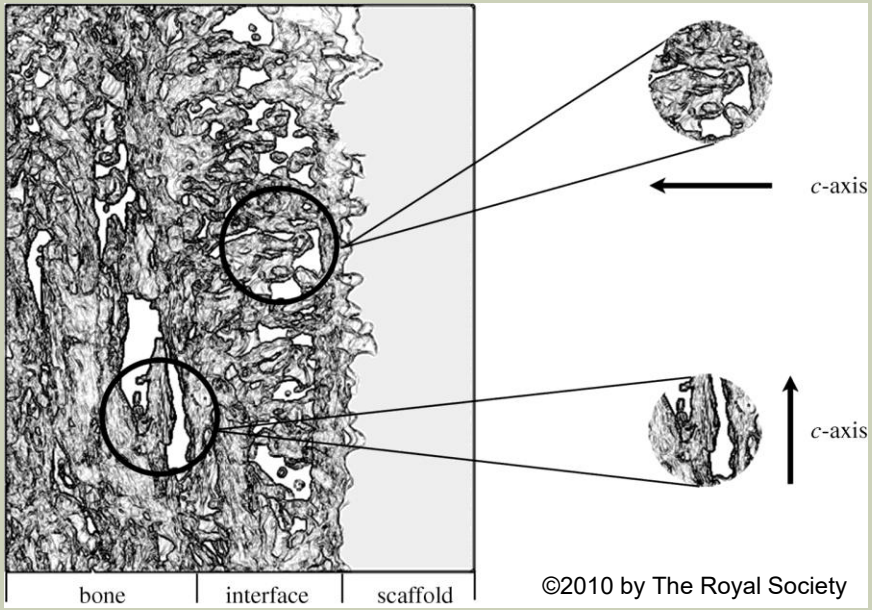


El hueso está formado a partes iguales (en volumen) por una proteína fibrosa estirable llamada colágeno y por una fase mineral quebradiza llamada hidroxiapatita.



El calcio se presenta en los huesos bajo la forma de hidroxiapatita fosfato de calcio cristalino [$Ca_{10}(PO_4)6(OH)_2$].

An illustration of the human bone–scaffold interface indicating the differences in HA crystal orientation visible with electron tomography.



Grandfield K et al. J. R. Soc. Interface
doi:10.1098/rsif.2010.0213

Los cristales más superficiales en el hueso están orientados con su eje largo (eje -c) paralelo a la superficie, mientras que los cristales en la apatita de la capa interfacial tienen su eje largo orientado de manera perpendicular a la superficie.

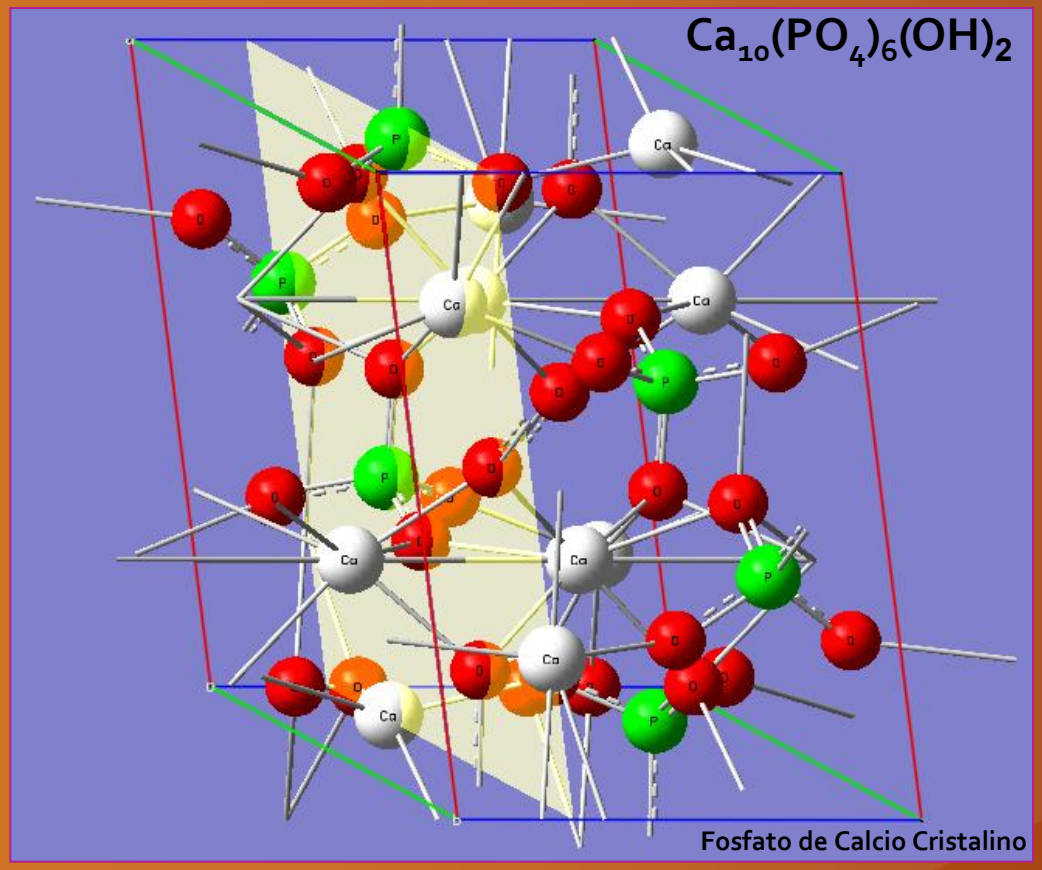
JOURNAL OF THE ROYAL SOCIETY Interface

CRISTAL DE HIDOXIAPATITA

Crystallography Open Database

COD ID: 4317043

Formula: - Ca10 H2 O26 P6 -
Comments: Lyudmyla I. Ardanova; Evgeni I. Get'man; Stanislav N. Loboda; Vadim V. Prisedsky; Tatiana V. Tkachenko; Valeriy I. Marchenko; Valeriy P. Antonovich; Nataliya A. Chivireva; Konstantin A. Chebishev; Alexandra S. Lyashenko Isomorphous Substitutions of Rare Earth Elements for Calcium in Synthetic Hydroxyapatites Inorganic Chemistry 49 (2010) 10687-10693
Space group: P 63/m
Cell volume: 528.69
Cell parameters: 9.41898; 9.41898; 6.88119; 90; 90; 120;



Tag*	Symbol	a	b	c
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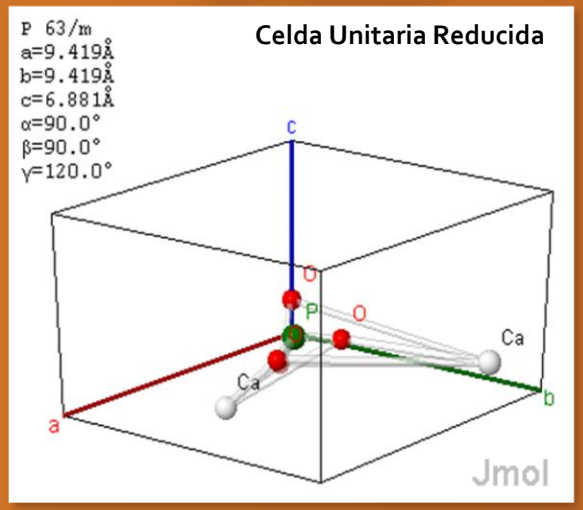
2	Ca	0.246300	0.992100	1/4
3	P	0.399100	0.369500	1/4
4	O	0.325800	0.489500	1/4
5	O	0.586600	0.464300	1/4
6	O	0.346400	0.259600	0.061400
7	O	0	0	0.182000
8	Ca	1/3	2/3	0.497000
9	Ca	1/3	2/3	0.003000
10	Ca	2/3	1/3	0.503000
11	Ca	0.254200	0.246300	3/4
12	Ca	0.007900	0.254200	1/4
13	Ca	0.753700	0.007900	3/4
14	Ca	0.745800	0.753700	1/4
15	Ca	0.992100	0.745800	3/4
16	P	0.029600	0.399100	3/4
17	P	0.630500	0.029600	1/4
18	P	0.600900	0.630500	3/4
19	P	0.970400	0.600900	1/4
20	P	0.369500	0.970400	3/4
21	O	0.836300	0.325800	3/4
22	O	0.510500	0.836300	1/4
23	O	0.674200	0.510500	3/4
24	O	0.163700	0.674200	1/4
25	O	0.489500	0.163700	3/4
26	O	0.122300	0.586600	3/4
27	O	0.535700	0.122300	1/4
28	O	0.413400	0.535700	3/4
29	O	0.877700	0.413400	1/4
30	O	0.464300	0.877700	3/4
31	O	0.086800	0.346400	0.561400
32	O	0.740400	0.086800	0.061400
33	O	0.653600	0.740400	0.561400
34	O	0.913200	0.653600	0.061400
35	O	0.259600	0.913200	0.561400
36	O	0.653600	0.740400	0.938600
37	O	0.913200	0.653600	0.438600
38	O	0.259600	0.913200	0.938600
39	O	0.346400	0.259600	0.438600
40	O	0.086800	0.346400	0.938600
41	O	0.740400	0.086800	0.438600
42	O	0	0	0.682000
43	O	0	0	0.818000
44	O	0	0	0.318000

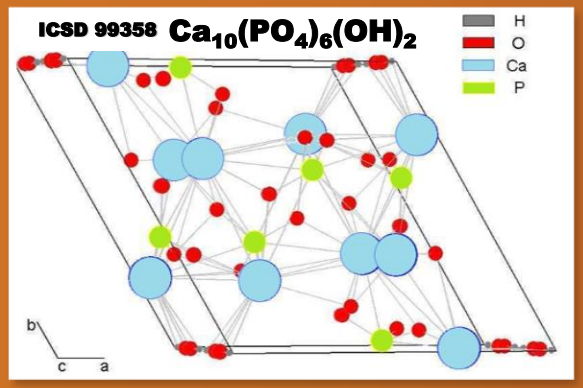
CRISTAL DE HIDOXIAPATITA

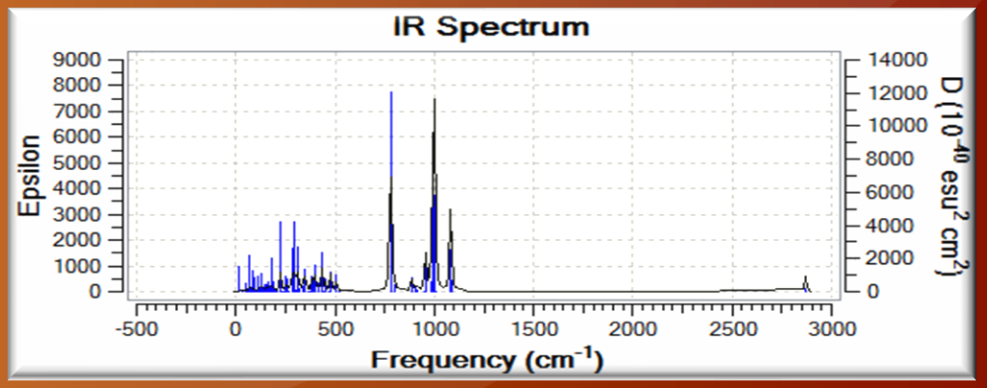
Crystallography Open Database



Structure parameters

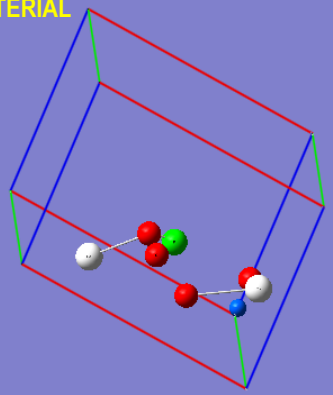
Formula	- Ca10 H2 O26 P6 -
Calculated formula	- Ca10 O26 P6 -
Authors of publication	Lyudmyla I. Ardanova
Journal of publication	Inorganic Chemistry
a	9.41898 ± 0.00019 Å
b	9.41898 ± 0.00019 Å
c	6.88119 ± 0.00017 Å
α	90°
β	90°
γ	120°
Cell volume	528.69 ± 0.02 Å³
Cell temperature	296 K
Ambient diffraction temperature	296 K
Number of distinct elements	4
Hermann-Mauguin symmetry space group	P 63/m
Hall symmetry space group	-P 6c
Residual factor R(I) for significantly intense reflections	7.7502
Goodness-of-fit parameter for all reflections	1.1644
Diffraction radiation wavelength	1.5418 Å
Diffraction radiation type	CuKα



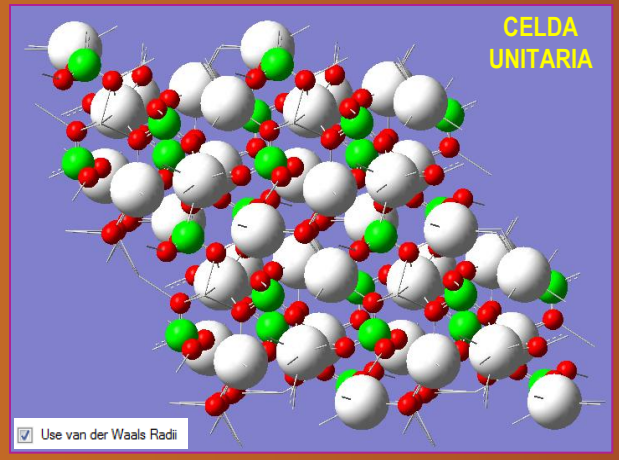


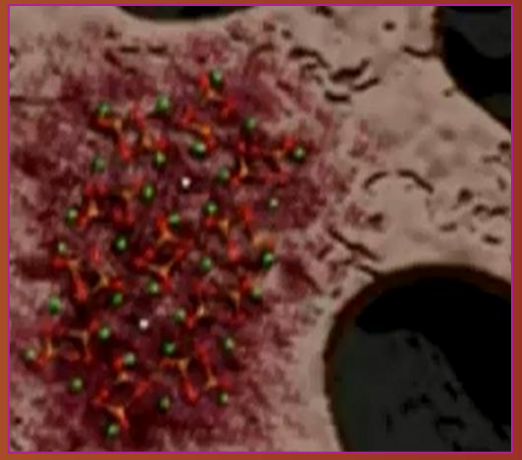
CRISTAL DE HIDOXIAPATITA

UNIDAD MÍNIMA DE MATERIAL
Coordenadas Reducidas



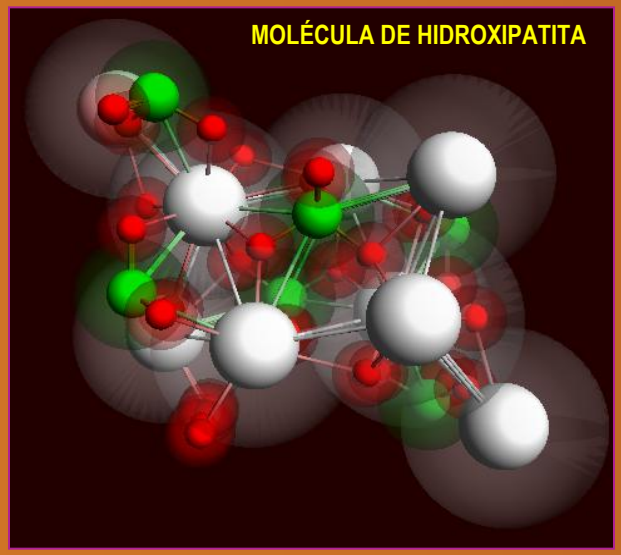
Ca	0.6666	0.3333	0.0016
Ca	-0.0070	0.2416	0.2500
P	0.3694	0.3984	0.2500
O	0.4859	0.3273	0.2500
O	0.4666	0.5882	0.2500
O	0.2575	0.3414	0.0707
H	0.0000	0.0000	0.2500

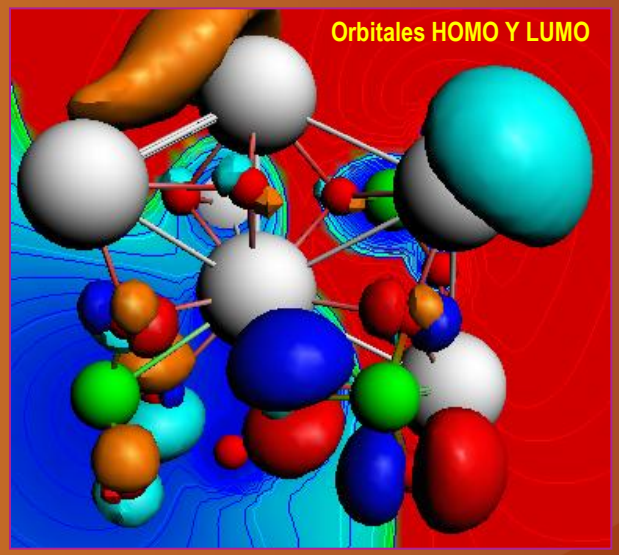


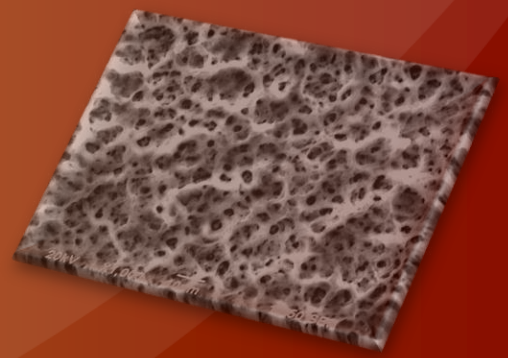


ESTRUCTURA MOLECULAR

El componente inorgánico de la matriz ósea está constituido en su mayor parte por fosfato cálcico en forma de cristales de hidroxiapatita.



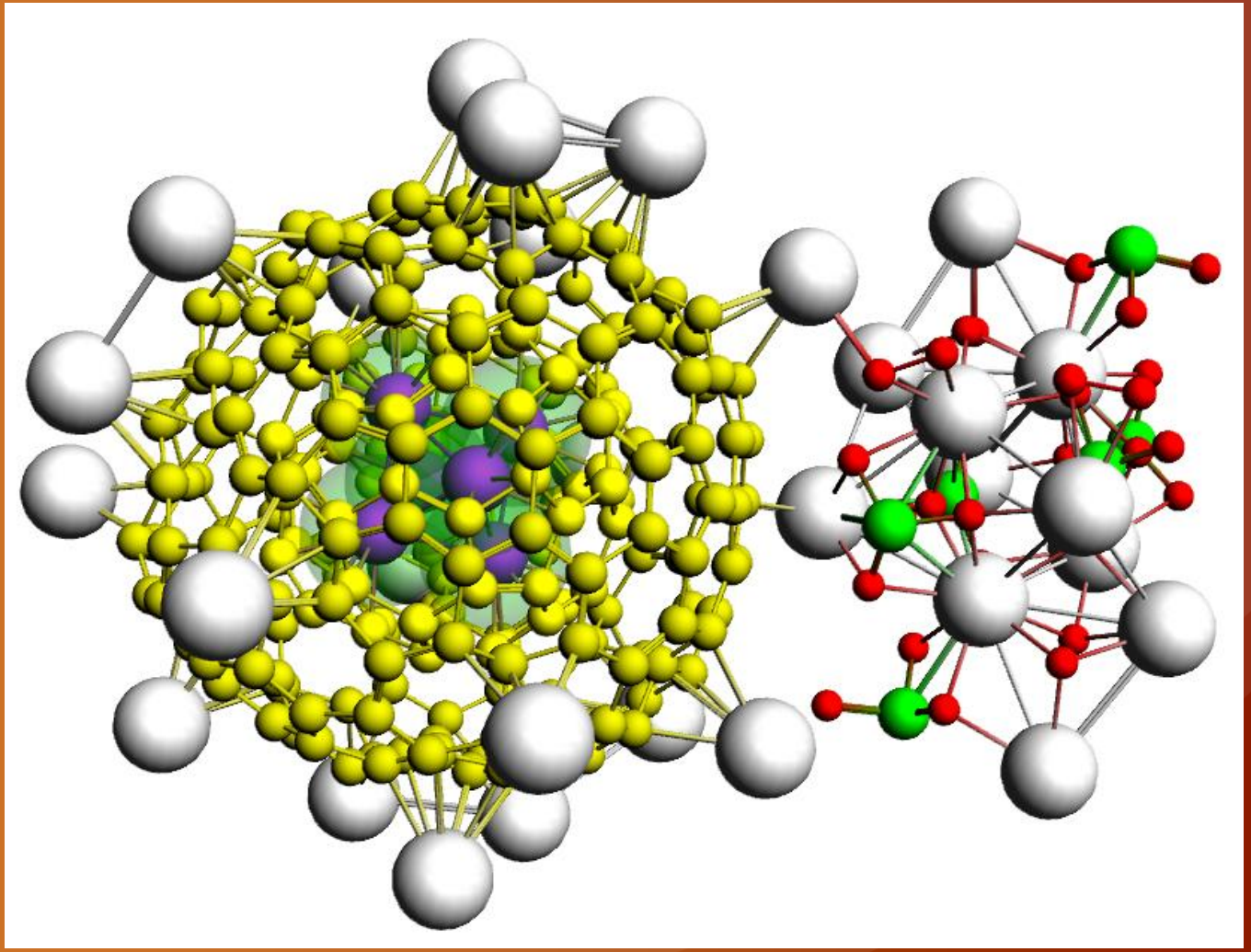




ESTRUCTURA MICROSCÓPICA

Ti5a (T=265°C, H_3PO_4=0.14% y Ca/P=1.00)

Interacción de una Nanocápsula Multicapa con una molécula de Hidroxiapatita



Agradecimientos

CICATA-Legaria, IPN

Supercómputo DGTIC, UNAM

Dr. José Guzmán Mendoza

CONACYT